

Modeling of nutrient dynamics during flood events at catchment scale in tropical regions

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Dedicated to my parents with love
Kính tặng cha mẹ vô vàn kính yêu

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Abstract

Water pollution is one of the biggest water-related problems. Water pollution threatens human livings as well as ecosystems. This problem is especially increasing in developing countries. Lack of knowledge and powerfull techniques are some typical reasons that make difficulties to protect water resources. Water quality modeling at catchment scale has been popularly used to assist water management in developed countries.

Thus, the aim of this dissertation is to study how catchment water quality modeling can be applied in the tropical conditions (e.g. Vietnam), especially looking at the aspect of transferring current knowledge from developed countries to developing countries. In order to achieve this aim, the PhD study conducts the following work: (1) review on the state of the art of water quality modeling at catchment scale; (2) selection of a suitable study area for testing and validating concepts; (3) utilization of available complex model codes; (4) development of an innovative and robust adapted to the specific condition of tropical regions in developing countries; (5) proposition of a model-based framework for water resources management. These five aspects are presented consequently from chapter 2 to chapter 6. Achieved results are presented in the following.

The review with focus on nutrient dynamics at small scale catchment includes

- Hydrological modeling
- Soil erosion and sediment transportation
- Nutrient forms, transformations and transports at catchment scale
- Flow and contaminant routing in river network
- Integrated water quality modeling and current modeling issues (ungauged catchment, scale, model complexity, model uncertainty).

Thus, an overview of catchment water quality modeling is given that will support for other steps in the later stage.

To test the different types of modeling, a small catchment in Vietnam, namely Tra Phi located about two hours North West from Ho Chi Minh City was used. The catchment is representative for typical problems in water quality pollution in Vietnam such as existing point and diffuse sources. Description of the catchment is provided in two aspects: Data collection and measurement of river discharge and water quality parameters performed as a part of this PhD thesis. Results show the importance of water quality monitoring during flood events. Existing point and diffuse sources were clearly observed. Monitoring of data is essential to assess the water quality of the catchment. Nevetherless, it is not enough in water management perspectives such as to trace water pollution sources or to develop water quality management schemes.

From the group of highly complex models being applied on a world-wide level, the HSPF (Hydrology Simulation Program – FORTRAN) model is selected and implemented for the pilot catchment. Results showed that although the model was successfully applied, many constrains occurred due to limited data, parameter uncertainty, expertise requirement etc. that make the model difficult to be used as an operational tool for the region. This aspect is considered as a motivation for developing a simpler yet accurate model for operational purposes for the region.

Consequently, the development and test of an event-based catchment water quality model SINUDYM (Simplified Nutrient Dynamics Model) is presented. The model aims to cope with practical issues (e.g. limited data, error propagation). Simplified model structure and limited model parameters are the most appealing features. All model components are coupled and controlled within one file. Similar to the output of the HSPF model and despite of its simplicity, the new model provided results which reasonably well show the nutrient dynamics in tropical regions.

Finally, a review on water quality management in Vietnam is provided before introducing a model-based water management framework. The framework comprises of (waste) load allocation, water pollution reduction, water quality monitoring, public participation, communication to decision-maker that all can be beneficial from modeling activities. Constrains for implementing models in water quality management in Vietnam were pointed out including improving monitoring data, expertise, modeling tools/guideline, small scale research study, public participation. In addition, recommended solutions for promoting models in water quality management are: developing model-oriented initiative; guidance for model development, implementation; joining integrated water resources management and adaptive water resources management.

The experience gained from modeling and the recommendations will be used in an ongoing joint research project (German Ministry of Education and Research – BMBF and Vietnam Ministry of Science and Technology – MOST) about “Water pollution control management in key economics zones of South Vietnam”. Coordinators of this project are the Leichtweiß-Institute for Hydraulics and Water Resources (LWI), University of Braunschweig and the Institute for Environment and Resources (IER), Vietnam National University of Ho Chi Minh city.

In conclusion, the PhD project has achieved a clear success in promoting water quality modeling at catchment scale for water resources management in tropical regions in particular in Vietnam. The work has gone through a process of learning, implementing, developing and testing catchment water quality models. Limitations of the work are also presented including, for example, improvement of data collection, consideration of uncertainty sources and analysis. Small scale catchment study, comparative study, GIS integration and adaptive water quality management are most-recommended subjects for further research.

Zusammenfassung

Die vorgelegte Doktorarbeit beinhaltet folgende Themen: (1) Eine Literaturstudie über den aktuellen Stand der Gewässergütemodellierung auf Einzugsgebietsebene; (2) Auswahl eines geeigneten Einzugsgebietes zum Testen und Validieren von Modellkonzepten; (3) Anwendung von vorhandenen komplexen Modellen; (4) Entwicklung eines innovativen, robusten und an die spezifischen Bedingungen tropischer Regionen angepassten Modellkonzeptes; (5) Vorschläge für ein modellbasiertes Wasserressourcenmanagementkonzept.

Der Schwerpunkt der Literaturstudie liegt auf der Modellierung der Nährstoffdynamik kleiner Einzugsgebiete und umfasst die Themengebiete: Hydrologische Modellierung, Bodenerosion und Sedimenttransport, Nährstofftransformation- und Transport auf Einzugsgebietsebene, Abfluss- und Schadstoffrouting im Flussnetz, integrierte Gewässergütemodellierung sowie aktuelle Themen der Einzugsgebietsmodellierung (Einzugsgebiete ohne Pegel, Skaleneffekte, Modellkomplexität, Modellunsicherheit).

Um die verschiedenen Modellansätze zu testen, wurde ein kleines Einzugsgebiet in Südvietnam ausgewählt. Das Einzugsgebiet ist repräsentativ in Bezug auf die typischen Umweltprobleme in Vietnam. Die nötigen Abfluss- und Gewässergütedaten wurden im Rahmen dieser Doktorarbeit erhoben. Die Messungen zeigen, dass das Gewässergütemonitoring während Hochwasserereignissen von großer Bedeutung ist. Vorhandene punktuelle und diffuse Nährstoffquellen wurden beobachtet. Das Monitoring ist unerlässlich, um die Gewässergüte im Einzugsgebiet zu ermitteln. Aber es ist nicht ausreichend um die Quelle der Verschmutzung zu identifizieren oder Managementpläne zu entwickeln.

Aus den weltweit eingesetzten komplexen Modellen wurde das Modell HSPF (Hydrology Simulation Program – FORTRAN) ausgewählt und erfolgreich auf das Modellgebiet angewandt. Allerdings ist HSPF, auf Grund der limitierten Datenverfügbarkeit und daraus resultierender Parameterunsicherheiten, nur bedingt als Managementwerkzeug in der Region anwendbar. Dieser Umstand wird als Motivation gesehen, einen einfacheren, auf die regionalen Bedingungen abgestimmten, aber dennoch ausreichend genauen Modellansatz zu entwickeln.

Daher wurde im Rahmen dieser Arbeit das eventbasierte, auf Einzugsgebietsebene agierende Stofftransport und Gewässergütemodell SINUDYM (Simplified Nutrient Dynamics Model) entwickelt und getestet. Das Modell zeichnet sich durch seine einfache Struktur und eine geringe Anzahl von Modellparametern aus. Alle Modellkomponenten sind in einer Datei gekoppelt und werden über diese gesteuert. Das Modell liefert im Vergleich zu HSPF gute Ergebnisse und bildet die Nährstoffdynamik im tropischen Einzugsgebiet, trotz seiner Einfachheit, sehr gut ab.

Die Erkenntnisse aus den Modellanwendungen sowie die Empfehlungen zum Managementkonzept werden in einem laufenden Verbundforschungsprojekt (Bundesministerium für Bildung und Forschung – BMBF und Vietnam Ministry of Science and Technology – MOST), über "nachhaltiges Gewässerschutzmanagement in der Hauptwirtschaftszone in Südvietnam", verwendet. Koordinator dieses Projektes ist das Leichtweiß-Institut für Wasserbau (LWI) der Technischen Universität Braunschweig und das Institute for Environment and Resources (IER), Vietnam National University of Ho Chi Minh city.

Abschließend erfolgte eine Literaturstudie über Gewässergütemanagement in Vietnam. Darauf aufbauend wurde modellbasiertes Wasserressourcenmanagementkonzept vorgestellt. Das Konzept beinhaltet Schadstoffeintrag, Verringerung des Schadstoffeintrags, Gewässergütemonitoring, Beteiligung der Öffentlichkeit, Kommunikation zwischen den Entscheidungsträgern. Die nötigen Randbedingungen, um Modelle im Gewässergütemanagement in Vietnam einsetzen zu können, wurden herausgearbeitet. Diese umfassen verbessertes Datenmonitoring, Expertenwissen, Modelltechnik und Richtlinien, kleinskalige Forschung und Beteiligung der Öffentlichkeit. Weitere empfohlene Maßnahmen zur Etablierung von Modellen im Gewässergütemanagement sind: Aufbau modellorientierter Unternehmen, Beratung zur Modellentwicklung und Implementierung sowie die Zusammenführung von integriertem und adaptiven Wasserressourcenmanagement.

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Abbreviation

ADCP	: Acoustic Doppler Current Profiler
ANGPS	: Agricultural Non-Point Sources
CN	: Curve Number
CNS	: Cornell Simulation model
CREAMS	: Chemicals, Runoff, and Erosion from Agricultural Management Systems
CSRT	: Continuous-Stirred Tank Reactor
d	: Agreement index
DEM	: Digital Elevation Model
DWSM	: Dynamic Catchment Simulation Model
ESWAT	: Extended Soil and Water Assessment Tool
ESWAT	: Enhanced Soil and Water Assessment Tool
GIS	: Geographic Information System
GIUH	: Geomorphologic Instantaneous Unit Hydrograph
GLEAMS	: Groundwater Loading Effects of Agricultural Management Systems
GLUE	: Generalised Likelihood Uncertainty Estimation
GPS	: Global Positioning System
GRIPs	: Geo referenced interface package for the AGNPS 5.0 catchment model
HBV	: Hydrologiska Byråns Vattenbalansavdelning
HRU	: Hydrologic Response Units
HSPF	: Hydrological Simulation Program - Fortran
ILWIS	: Integrated Land and Water Information System
IWRM	: Integrated Water Resources Management
m.a.s.l	: meter above sea level
MCMC	: Monte Carlo Markov Chain
MONERIS	: Modeling Nutrient Emission in River Systems
MONRE	: Ministry of Natural Resources and Environment
MUSLE	: Modified Universal Soil Loss Equation
NA	: Not applicable
NPSM	: Non Point Sources Model
NSE	: Nash-Sutcliffe efficiency
PBIAS	: Percent bias
pdf	: Probability density function
PE	: Potential evaporation
PET	: Potential evapotranspiration
QUAL2	: Enhanced Stream Water Quality Model
QUALOF	: Ovelandflow associated constituents (in HSPF model)
QUALSD	: Sediment associated constituents (in HSPF model)
R2	: Coefficient of determination
RA	: Area ratio
RB	: Bifurcation ratio
RL	: Length ratio
RMSE	: Root Mean Square Error
RS	: Remote Sensing
RUSLE	: Revised Universal Soil Loss Equation
SCS	: Soil Conservation Service
SCS CN	: Soil Conservation Service Curve Number
SHE	: Système Hydrologique Européen

SINUDYM	: Simulation Nutrient Dynamic Model
SWAT	: Soil and Water Assessment Tool
TMDL	: Total Maximum Daily Load
USLE	: Universal Soil Loss Equation
VEA	: Vietnam Environment Administration
VEPA	: Vietnam Environmental Protection Agency
Vs.	: Versus
WaSiM-ETH	: <u>W</u> asserhaushalts- <u>S</u> imulations- <u>M</u> odell – <u>E</u> idgenössischen <u>T</u> echnischen <u>H</u> ochschule Zürich
WEPP	: Erosion Prediction project

1. Introduction

1.1. Introduction

“Water is essential for life.” We are all aware of its necessity, for drinking, for providing food, for washing, etc. – in essence for maintaining our health and dignity. Water is also required for providing many industrial products, for generating power, and for moving people and goods – all of which are important for the functioning of a modern, developed, and developing society. In addition, water is essential for the integrity and sustainability of the Earth’s system” (UN, 2003).

However, water availability is very concerned in the last decades. Demand and competition for water resources continue to grow almost everywhere. The main reason can be explained by the increase of the world population leading to higher demand on water in many activities such as agriculture, industry, energy supply, etc. In addition, especially, given the problem of climate change, water-related problems such as flood, drought, and water pollution are increasingly becoming challenging issues in the years to come (Biswas et al., 2005).

Water pollution is one of the biggest water-related problems. Water pollution threatens human livings as well as ecosystems. Excessiveness of nutrients in aquatic environment is a typical example of water pollution caused by various anthropogenic factors (e.g. industrial and urban wastewater, agricultural runoff). Eutrophication can be seen a consequence of excessive nutrients. It can lead to many environmental problems such as limited water supply, anoxia severely destroying aquatic ecosystem (e.g. decreasing fish, and other animal populations) through the food chain, water pollution can cause serious diseases to people (e.g. cancer) (Loague and Corwin, 2005; Novotny, 2002).

Many organizations appeal to solutions on this problem, especially the United Nations (UNCED, 1992). Approaches ranging from traditional top-down water resources management to “Integrated Water Resources Management (IWRM)” (Global Water Partnership, 2003; Zaag, 2005) or adaptive water management (Pahl-Wostl, 2007; Shabman et al., 2007) have shown certain successes and improvements in developed countries. Advances are, however, still very limited in developing countries (Biswas et al., 2005; García, 2006; Ujang and Buckley, 2002). Constrains due to pressure of economical development, lack of human resources, techniques and data are some common reasons found in these countries.

Allan (2003) presents five water management paradigms through more than one hundred years. From the Figure 1.1, we can think that many countries are now in the 5th paradigm, but there are still many other countries in the 3rd, 4th or 2nd paradigms. Based on the author’s experience, Vietnam is now at the beginning of the 4th paradigm. It can be assumed that there is an opportunity to transfer management knowledge from the developed world to the developing world in order to improve water management. For example, Malano et al. (1999) state “*it is often observed that the problems preoccupying developed countries are not entirely different in nature from those that focus attention of developing countries*”. Therefore, bringing good tools and techniques (i.e. knowledge) which are successfully implemented in developed countries to developing or emerging countries is an interesting approach.

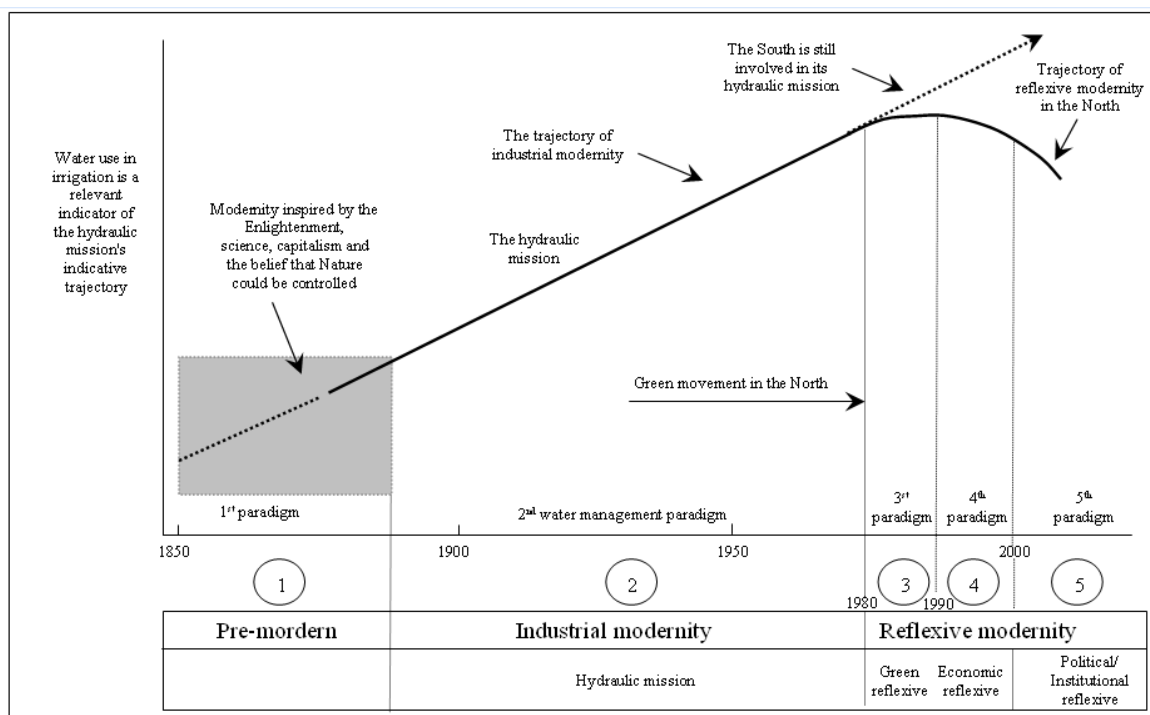


Figure 1.1: Five water management paradigms 1850-2000 (Allan, 2003)

In Vietnam, water resources management is facing many challenges. Water pollution is becoming one of the greatest concerns in the country (VEA, 2009; VEPA, 2005). Although the IWRM has been introduced and regulated in some legal document, success in water resources management is still rather limited (Global Water Partnership, 2003; Hansen and Do, 2005). Typical reasons are related to the management of pollution sources. While controlling pollution caused by point-sources is still rather difficult, diffuse sources are mostly ignored in water quality management plan. Further reasons are the limited human resources and the lack of monitoring data. There is an urgent need of a powerful tool required to improve water resources management.

Catchment water quality modeling has being shown as a useful tool for water quality management. It is widely applied in many water quality management programs, such as the Total Maximum Daily Load (TMDL) in the United States of America (NRC, 2001) or in the Water Framework Directive in the European Community (Hattermann and Kundzewicz, 2009). The catchment water quality model or, in short, catchment model, adapts a catchment at a model scale. The physical, chemical and biological processes occurring in the catchment as well as the anthropogenic factors can be included in the model so that many management schemes can be tested and implemented. Therefore, it can be used to assist water managers in giving effective decisions for water protections.

1.2. Objective and approach of the study

The overall aim of this research study is to explore how modeling can effectively assist water quality management. Modeling nutrient dynamics at catchment scale in sub-humid tropical conditions with focus on Vietnam is considered as a case study. To achieve this aim, the following five steps are performed:

- To analyse nutrient dynamics processes at catchment scale and to model these processes
- To select a suitable area as a pilot catchment

- To select and implement available complex model codes
- To develop and test a new model, which account for the specific constraints, demands of tropical regions in developing countries
- To develop a strategy for utilizing models in water quality management in Vietnam

These five steps are presented in chapter 2 to chapter 6 as shown in Figure 1.2

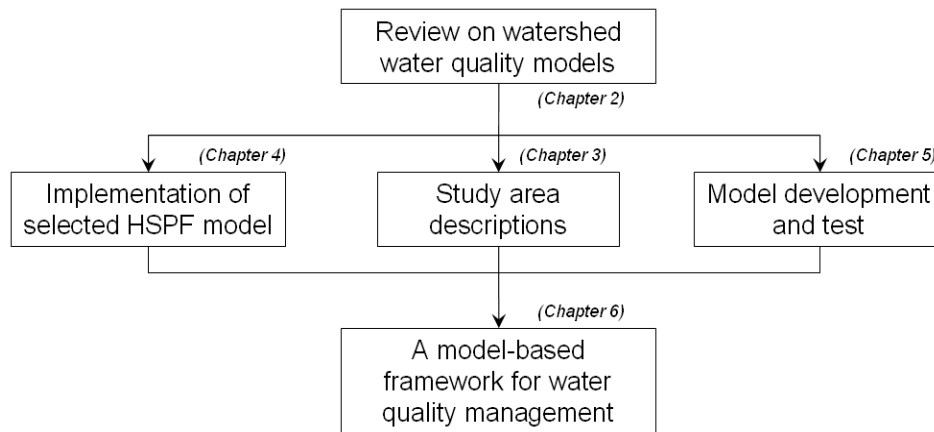


Figure 1.2: Study approach

It is intended to include the findings of this thesis into an ongoing joint research project financed by the German Ministry of Education and Research – BMBF and Vietnam Ministry of Science and Technology – MOST about “Water pollution control management in key economics zones of South Vietnam”. Coordinators of this project are Leichtweiß-Institute for Hydraulic Engineering and Water Resources (LWI), Technical University of Braunschweig and the Institute for Environment and Resources (IER), Vietnam National University of Ho Chi Minh city (Meon and Le, 2010).

1.3. Impacts of the study

It is very clear that there is a big gap in water resources management between developed and developing countries. Vietnam has been facing with water pollution in the recent decades. Finding suitable tools developed and successfully used and applying them in Vietnam is very essential. This aspect can be regarded as the win – win situation since the country can be beneficial from the advanced knowledge, meanwhile the knowledge can be applied in a specific condition (Schöniger, 2009). Therefore, this dissertation will contribute to the following aspects:

- Transferring knowledge to practical problems in developing countries
- Characterising specific conditions of sub-tropical regions, e.g. Vietnam
- Promoting catchment water quality modeling as a useful tool for water quality management.

1.4. Thesis outline

The thesis comprise of 7 chapters. The core works are from chapter 2 to chapter 6, while chapter 1 and chapter 7 are the introduction and conclusion, respectively.

- Chapter 2: Review on the state of the art of catchment water quality modeling with emphasize on nutrient dynamics is provided.
- Chapter 3: Descriptions of the study area, Tra Phi catchment and the data collection for the model simulation are given
- Chapter 4: The implementation and application of the selected Hydrologic Simulation Program – Fortran (HSPF) for the Tra Phi catchment is described.
- Chapter 5: A newly-developed model in order to cope with the specific regional problems is presented.
- Chapter 6: A review on how model can be instrumental to water quality management is provided. It is followed by point out constrains for utilizing catchment water quality model in Vietnam. Solutions for promoting model application and development in Vietnam are introduced with a focus on a model-based framework for catchment water quality management.

2. Review on water quality modeling at catchment scale

First, the physically-driven processes are described in sections 2.1 and 2.2: catchment hydrology, and soil erosion, respectively. Next, nutrient transport and transformation of nitrogen and phosphorus within a catchment will be presented in sections 2.3 and 2.4, respectively. Flow, sediment, and contaminants routing in rivers will be discussed in the section 2.5. The state of the art of approaches in water quality modeling at catchment scale is also reviewed. Finally, some remaining issues as well as relevant approaches for this study are considered.

2.1. Catchment hydrology

2.1.1. Catchment hydrology cycle

Catchment hydrology is a key unit that should be understood in order to properly manage water resources (Singh, 1995b). The catchment hydrology cycle is presented in the following paragraphs.

The catchment hydrologic cycle involves many interacting processes. A summary of the cycle is given by Chow et al (1988). Detailed descriptions can be found in Kirby (1978). The processes are illustrated in Figure 2.1 and Figure 2.2.

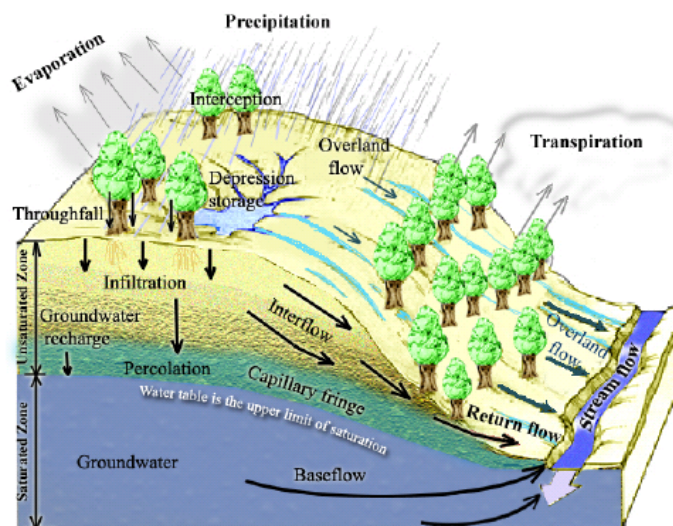


Figure 2.1: Physical processes involved in Runoff Generation (Tarboton, 2003)

Precipitation is the most essential factor for the generation of runoff at a catchment scale. The distribution of precipitation varies spatially and temporally in the nature. Precipitation can be in the form of snow, hail, dew, rain and rime (Bras, 1990). In this study, precipitation is considered in the form of rain only.

Rainfall travels in a catchment in different directions. Due to vegetation, part of the rainfall is intercepted by vegetation canopy. *Interception* is known as a loss function to catchment runoff depending on vegetation type and vegetation density. The rest of the rainfall moves down the vegetation as stem flow; dripping off the leaves, or directly falling to the ground as throughfall. Remaining rainfall remains at the land surface as depression storage will either evaporates, infiltrates or is discharged as overland flow.

Infiltration of rainwater occurs when the water moves primarily in a downward direction by unsaturated subsurface flow and recharges the saturated zone. This process is termed *groundwater recharge* or *percolation* or *natural recharge* when water fills the aquifers of groundwater system. In some cases at the shallow subsurface layer, where the lateral hydraulic conductivity is higher than the vertical one, the direct infiltration partially goes toward the channel through *interflow* or *throughflow*.

The groundwater pattern is influenced by the catchment characteristics, especially the topographic factors and soil characteristics, before being discharged to the channel network system. Aquifers of the groundwater system also can discharge groundwater across the catchment boundary, even though this is not depicted in the figures.

Evapotranspiration is a term for *evaporation* and *transpiration* at the land surface causing a decrease of water storage in the subsurface. As a consequence, unsaturated flow in upward direction is generated in a *capillary rise process*. In Figure 2.2 evaporation from channel is omitted.

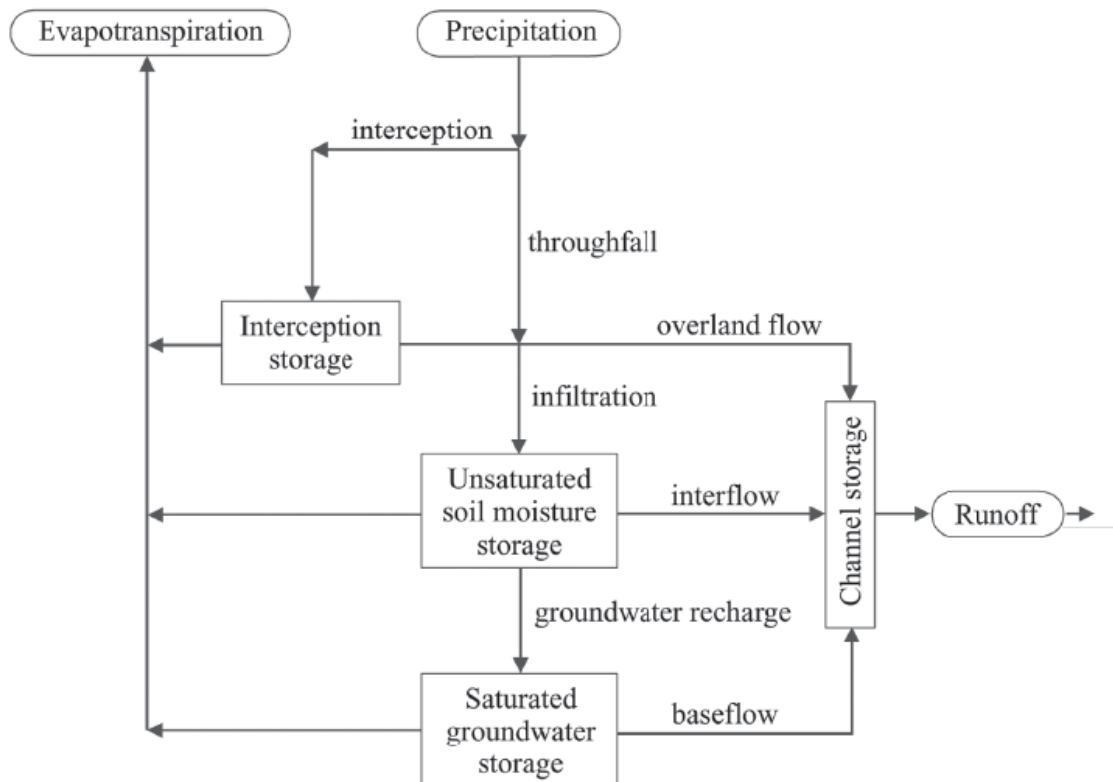


Figure 2.2: Network model of part of hydrological cycle (Freeze and Cherry, 1979, cited in Carrera et al., 2005)

2.1.2. Catchment runoff generation

Catchment runoff is the most observable component in catchment hydrology cycle, i.e. the transformation of river discharge at the catchment outlet. A quantitative assessment of the catchment runoff requires understanding of the mechanism of *runoff generation or streamflow generation* (e.g. see Beven, 2006). This topic is discussed by a number of authors, for example, publications by Dunne (1983). Basically, the runoff generation at a catchment scale in general or hillslope scale in particular includes 2 main components: (1) surface flow and (2) subsurface flow. There are a number of flow processes within each main component as illustrated in Figure 2.2 and more detailed in Figure 2.3.

Surface flow: Surface flow processes include overland flow and river flow including stream flow and channel flow. The overland flow is known as *infiltration-excess overland flow* (Horton overland flow) or *saturation overland flow* (Dunne flow). The Horton overland flow is generated when the rainfall intensity exceeds the infiltration capacity of the soil, while the saturation overland flow is developed by a saturation mechanism where the soil becomes saturated by the perennial groundwater rising to the surface or by lateral or vertical percolation above an impeding horizon (Dunne, 1983). The overland flow is observed as sheet flow which then generates rill flow. A number of the rill flows will contribute or create the *stream flow* and later converge into *channel flow*.

Subsurface flow: Subsurface flow processes include unsaturated subsurface flow, perched subsurface flow, macro pore flow and groundwater flow. Subsurface runoff is generated as water is discharged from the surface into the subsurface system. The *unsaturated subsurface flow* is mostly in the vertical direction while the *perched flow* moves in lateral direction. The perched flow is generated when the shallow soil layer has a higher hydraulic conductivity as compared to the lower one. The *macro pore flow* occurs where the subsurface system has macro pores such as voids, natural pipes, cracks; the flow rapidly contributes to the groundwater system. *Ground water flow* is produced in the saturated zone which is fed through percolation of infiltrated water or from neighbouring system. The ground water contributes to the *channel flow* as *rapid groundwater flow* in the upper part of the initially unsaturated subsurface domain or as *delayed groundwater flow* in the lower part of the saturated subsurface domain.

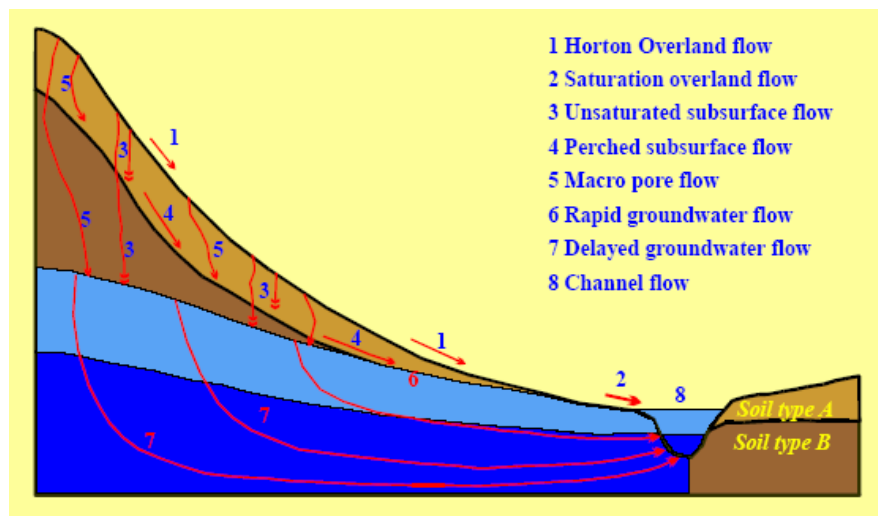


Figure 2.3: Cross-sectional presentation of hillslope flow process (after Rientjes, 2004) or simplified version in Dunne and Leopold (1978)

Although detailed processes of catchment hydrology have been comprehensively investigated, usually only a part of these processes are focused on in a research project. The reasons are (1) technical difficulty in looking at all processes, and (2) dominant mechanisms may be different at different physical settings (e.g. climate, topology) (e.g. see Dubreuil, 1985). Dunne (1983) conducted a review of runoff generation and its relationship with climate, land cover, land use, soil and topologic factors and catchment areas (see Figure 2.4). A hillslope may generate only subsurface flow during a gentle rainstorm, and Horton overland flow during a deluge (extreme rainfall); or subsurface flow alone during a short rainstorm and saturation overland flow during a long one. The variable source concept (Hewett and Hibbert, 1963) in Figure 2.4 is used to describe the temporal and spatial dynamics of the subsurface flow in relation to the saturation overland flow (Dunne, 1983; Dunne and Black, 1970).

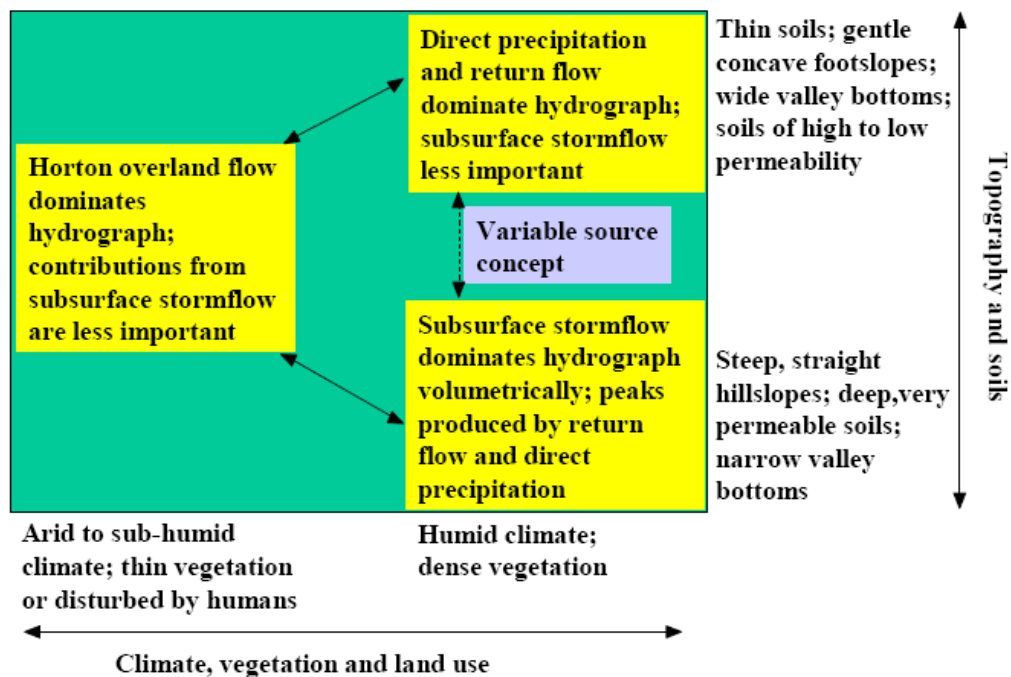


Figure 2.4: Schematic illustration of the occurrence of various runoff processes in relation to their major controls (Dunne, 1983; Dunne and Leopold, 1978)

2.1.3. Modeling approaches

The processes described earlier are not easy to quantify because most hydrologic systems are extremely complex. Abstractions of the processes are required instead of presenting them in detail. Modeling approach in catchment hydrology is used for this purpose. It is usually described in form of rainfall – runoff modeling.

In order to simulate the transformation from rainfall to runoff, rainfall – runoff models have been developed a long time ago. Reference is made to Todini (Todini, 1988; Todini, 2007) for historical review of rainfall - runoff modeling, or Singh and Woolhiser (2002) for review on catchment models. With respect to the development over the past decade, much efforts have been devoted to this issue as written by Beven (2000): “it is now virtually impossible for any one person to be aware of all the models that are reported in the literature”. In the following sections, most mathematical expressions are often used to describe catchment hydrology processes.

2.1.3.1. Water balance equation at catchment scale

The hydrological processes at catchment scale have been provided above. For modeling purposes, these processes should be presented in mathematical forms. A simple water balance equation describing the relationship between hydrological components is shown below:

$$\frac{\partial S}{\partial t} = P + G_{in} - (Q + ET + G_{out}) \quad (\text{eq. 2.1})$$

Where:

- S = Storage
- P = Rainfall
- G_{in} = Groundwater inflow
- Q = Runoff outflow
- ET = Evapotranspiration
- G_{out} = Groundwater outflow

At steady – state, $\frac{\partial S}{\partial t} = 0$, equation 2.1 becomes

$$P + G_{in} = (Q + ET + G_{out}) \quad (\text{eq. 2.2})$$

2.1.3.2. Runoff generation – the Soil Conservation Service method

The Soil Conservation Service (SCS) method was developed based on water balance equation as well as intensive experiments (Chow et al., 1988; Ogrosky and Mockus, 1964). In this method, rainfall excess and water loss in soil are lumped within a land-use unit. The most important aspect of the SCS method is the derivation of the Curve Number (CN). The CN is related to land use and soil characteristics that are listed in the SCS table. The CN values of each spatial unit are aggregated for the whole catchment by mean of the Geographic Information System (GIS) so that the average CN is obtained. The direct runoff or the effective rainfall is calculated using the following formula:

$$P_e = \frac{(P - 0.2S)^2}{P + 0.8S} \quad (\text{eq. 2.3})$$

For $P > 0.2 S$, and $P_e = 0$ if $P < 0.2 S$

Where:

- P_e = Effective rainfall or direct runoff expressed as a depth (mm)
- P = Total observed rainfall (mm)
- S = Potential maximum retention (mm)

$$S = \frac{25,400}{CN} - 254$$

2.1.3.3. Green-Ampt method for infiltration

Infiltration process can be modelled using different approaches such as the Horton's equation, or Philip's equation. This section uses the Green – Ampt method to describe infiltration process since it is the best approximation to the physical system (Chow et al., 1988). This method is derived from Darcy's equation and continuity principle. The final formula is as follows (Chow et al., 1988):

Cumulative infiltration, $F(t)$:

$$F(t) - \Delta\theta \ln \left[1 + \frac{F(t)}{\psi \Delta\theta} \right] = K(t) \quad (\text{eq. 2.4})$$

Infiltration rate, f :

$$f = K_s \left[\frac{\psi \Delta\theta}{F(t)} + 1 \right] \quad (\text{eq. 2.5})$$

Where:

- K = Hydraulic conductivity
- η = Porosity
- ψ = Wetting front suction head
- $\Delta\theta$ = $\eta - \theta_i$
- θ_i = Initial moisture content (dimensionless)

Variables in the Green – Ampt model are illustrated in Figure 2.5

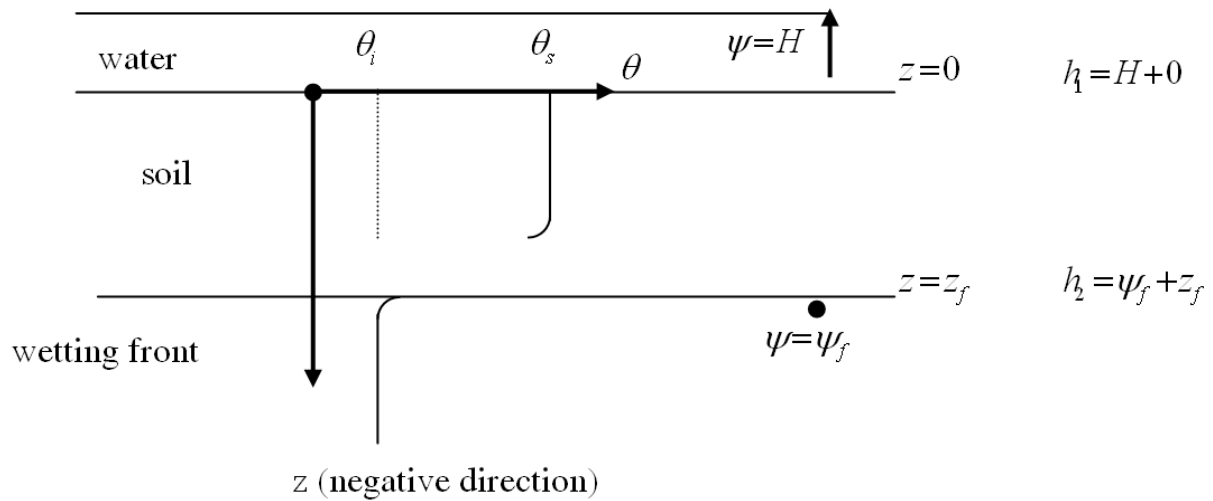


Figure 2.5: Variables in the Green – Ampt infiltration model (Chow et al., 1988)

Where:

- H = Depth of ponding (cm)
- K_s = Saturated hydraulic conductivity (cm/s)
- q = Flux at the surface (cm/h) and is negative
- ψ_f = Suction at wetting front (negative pressure head)
- θ_i = Initial moisture content (dimensionless)
- θ_s = Saturated moisture content (dimensionless)

2.1.3.4. Subsurface flow

Sub-surface flow can be expressed either by a simple empirical exponential recession equation or by combined-complex equations based on Darcy's law and on the continuity equation. A presentation of the Darcy law in one vertical direction is:

$$q = -K \frac{\partial h}{\partial z} \quad (\text{eq. 2.6})$$

Where:

- q = Flow (flux)
- K = Hydraulic conductivity
- h = Total head of flow
- '-' = Negative sign indicates the total head decreasing in the direction of flow (z)

2.1.3.5. Kinematic wave equation for overland flow

Kinematic wave equations consist of the continuity equations and the simplest form of the momentum equation after ignoring all the acceleration and pressure gradient terms in the Saint-Venant equation, respectively expressed as:

$$\text{Continuity equation: } \frac{\partial Q}{\partial x} + \frac{\partial h}{\partial t} = q \quad (\text{eq. 2.7})$$

$$\text{Momentum equation: } S_0 = S_f \quad (\text{eq. 2.8})$$

Detailed descriptions of these formulas are presented in section 2.5.1, "River routing". Overland flow can also be modelled using empirical approach where peak flow and time lags are estimated based on catchment morphology information, e.g. "Ungauged Basin Analysis" (U.S. Army Corps of Engineers, 1994)

2.1.3.6. Evaporation and evapotranspiration

Evaporation and evapotranspiration (combined evaporation from soil and transpiration from vegetation is another water loss from the catchment. The calculation is usually based on meteorological observations (e.g. radiation, wind velocity, air temperature). References on this topic are given by Allen et al. (1998) and Chow et al. (1988) and are omitted here. The calculation is often done at meteorological stations and used as input data for models.

2.2. Soil erosion

Soil erosion occurs when soil is detached by erosive agents like raindrop, surface water flow, and is later transported or deposited over the land surface¹. Because of erosion, billions tons of soils are lost annually in the world (e.g. approximately 5 billions tons of soil eroded every year in America (2001)) that is also equivalent to billions of US dollars. In addition, eroded soils carry (hazardous) pollutants to water bodies that are harmful to the aquatic ecology and to human beings (Nearing et al., 2001). According to the United States Department of Agriculture (USDA), soil erosion is the source of 80% of the total phosphorus, and 73% of the total Kjeldahl nitrogen in the waterways of the US., resulting in water-related problems (Julien, 1995; Lal, 1990; Morgan, 2005; Nearing et al., 2001; Novotny and

¹ Erosion caused by wind and irrigation activities is ignored in this dissertation

Chesters, 1981). Novotny (2002) lists a number of problems concerning erosion and sedimentation summarized as follows:

- Excessive sediment loading on receiving waters deteriorate aquatic habitats
- Excessive sedimentation causes a rapid loss of storage capacity in reservoirs and accumulation of bottom deposits which inhibit normal biological life
- Nutrients carried by the sediment can stimulate algal growths and, consequently, accelerate the process of eutrophication
- Sediment, especially its fine fractions, is a primary carrier of other pollutants, such as organic components, metals, ammonium ions, phosphates and many toxic organic compounds
- Erosion of streambanks and adjacent areas caused by the change in hydrology of urban catchment, destroy streambank vegetation that provides aquatic and wildlife habitat
- Turbidity from sediment reduces in-stream photosynthesis, which may lead to reduced food supply and habitat

Rose (1993) looks at the effects of soil erosion and sedimentation according to on-site and off-site as shown in Table 2.1

Table 2.1: Examples of on-site and off-site damage associated with water erosion and sedimentation

On-site	Off-site
Loss of plant nutrients	Siltation of stream, rivers, estuaries
Loss of organic matter	Siltation of Dam
Damage to soil structure	Damage to crops, roads, culverts, etc.
Subsoil Exposure	Deposition of soil pollutants

In this section a brief introduction to water erosion processes is presented, and then some important terminologies related to soil erosion are discussed, i.e. erosivity, erodibility, transport capacity, and sediment delivery ratio. Finally, physical processes of soil erosion, sediment yield and prediction methods are described.

2.2.1. Introduction

Soil erosion by water involves a number of factors or processes. First, because of the impact of rain drops, soil particles are detached (“splash effect”). When the soil exceeds its infiltration capacity or is saturated, overland flow occurs (see section 2.1). The overland flow can not only transport soil materials but can also detach soil particles. Soil erosion happens in the upland areas and can conceptually be regarded as interrill and rill erosion, where the first is smaller in unit as compared to the second (see Figure 2.6). The eroded materials are transported, deposited or re-detached other soil particles along the flow paths (i.e. channel networks). During these processes, factors that cause erosion (erosive factors) are expressed as erosivity, while other factors relating to the soil resistance to detachment and transportation are grouped as erodibility. Other catchment characteristics involving in soil erosion processes like slope and land cover are also considered (Figure 2.7)

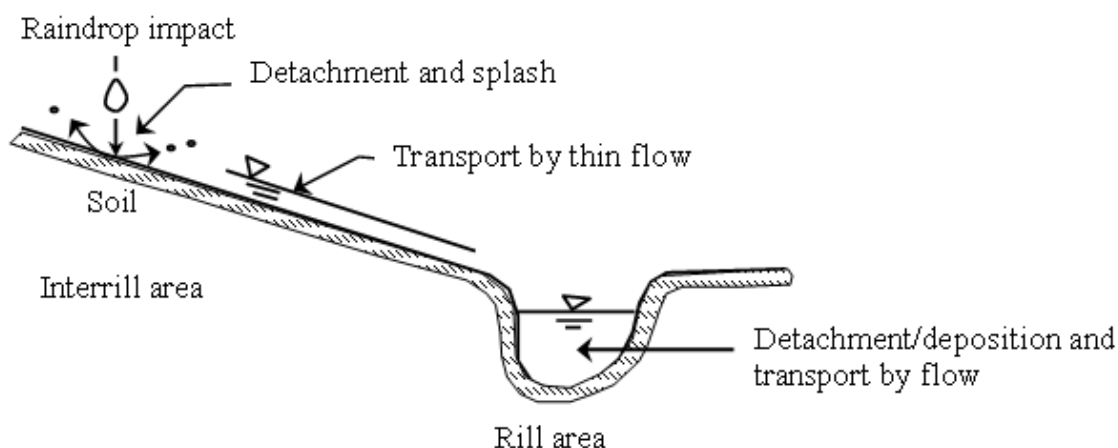


Figure 2.6: Erosion and transport on inter-rill and rill areas (Harmon and Doe, 2001)

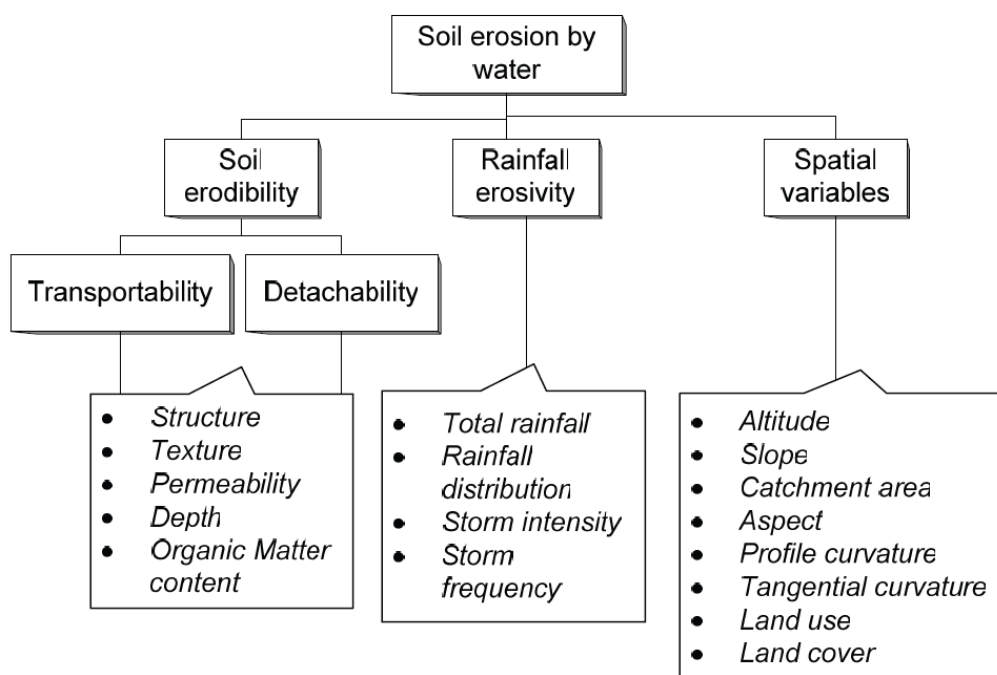


Figure 2.7: The main factors controlling the processes of soil erosion by water (Symeonakis, 2001, cited in Saavedra, 2005)

2.2.1.1. Erosivity of waters

Lal and Eliot (1994) define erosivity as an expression of the ability of erosive agents, like water, to cause soil detachment and transport.

Rainfall is considered the most erosive factor and followed by surface water. The term “splash erosion” is implied for erosion caused by rainfall because a rain drop splashes soil or detaches soil

particles by impacting rain drop (Lal, 1990). The rainfall characteristics and its kinetic energy (KE)² are often used to assess the erosivity.

Wischmeier and Smith (1958, cited in Morgan, 2005) propose:

$$KE = 0.0119 + 0.0873 \log_{10} I \quad (\text{eq. 2.9})$$

Where:

I = Rainfall intensity (mm/h)
 KE = Kinetic energy (MJ/ha/mm)

However, rainfall characteristics are different from region to region and its erosivity also varies significantly. Morgan (2005) reports the erosivity threshold in tropical (semi-arid, and semi-humid) areas as 25mm/h, which is much higher than the 1-10mm/h in the temperate region (e.g. Western Europe). Thus, Hudson (1965, cited in Morgan, 2005) provides another formula to calculate the KE for tropical countries:

$$KE = 0.298 \left(1 - \frac{4.29}{I}\right) \quad (\text{eq. 2.10})$$

Overland flow erosivity is complex and difficult to define precisely (Lal, 1990). Flow velocity and its related shear force detach the soil particle, and then the detached particles are transported by flowing water. The erosivity of surface flow has a smaller impact comparing to the splash effects. However, the detachment caused by the shallow flow increases exponentially with the slope angle up to a critical angle, where the flow changes from sheet to rill flow (Lal, 1990). Horton overland flow (as mentioned in the previous section 2.1) is usually the only component considered as erosive agent (beside rain drop) in soil erosion models.

2.2.1.2. Soil erodibility

Erodibility, a soil characteristic, is a measure of the soil's susceptibility to detachment and transport by the agents of erosion (Lal and Eliot, 1994). Morgan (2005) defines erodibility as the resistance of the soil to both detachment and transport. Although soil's resistance to erosion depends partly on topographic position, slope steepness and the amount of disturbance, such as during tillage, the properties of the soil are also important determinants. Erodibility varies with soil texture, aggregate stability, shear strength, infiltration capacity and organic and chemical content.

K is the most popular index expressing the soil erodibility. As presented in the above definition, when computing or estimating K value, a number of factors are take into account, e.g. soil texture, organic percent, soil structure and permeability. See Figure 2.8 for an example of implementing the Universal Soil Loss Equation (USLE)³.

² $KE = \frac{1}{2} mv^2$ (J), m: mass (kg); v: velocity (m/s)

³ The USLE will be explained in the next parts.

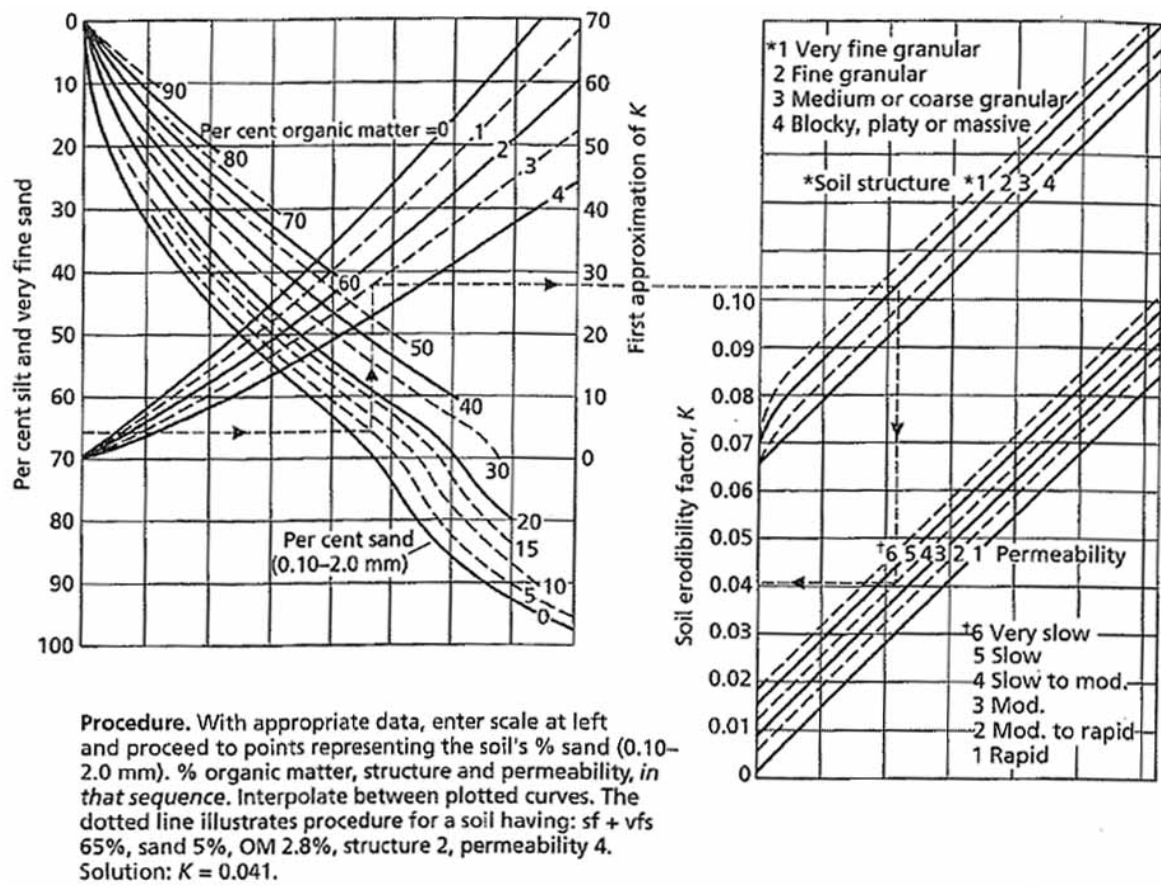


Figure 2.8: Nomograph for computing the K value (metric units) of soil erodibility for use in the Universal Soil Loss Equation (Wischmeier et al, 1971, cited in Morgan, 2005)

2.2.1.3. Sediment transport capacity

Nearing et al. (2001) distinguish soil and sediment for clarity as follows: “Soil is considered, for modeling purposes, to be material that is in place at the beginning of an erosion event. If the soil material is detached during an event, it is considered to be sediment”. The sediment transport capacity is equal to the maximum amount of sediment carried by flowing water without deposition. Thus, the sediment supply and sediment transport capacity is inter-related. When sediment supply is less than transport capacity then the transported materials is limited by the detachment capacity (maximum sediment supply – supply limited). In contrast, when the detachment capacity is greater than the transport capacity, the transport capacity limits the amount of eroded materials that can be transported (capacity limited). Julien (1995) proposes the relation among the sediment transport capacity and sediment supply and, especially, with particle sizes as shown in Figure 2.9. Here, the *washload* is the sediment moving at the water surface and supported mainly by the turbulence of the flow, and the *bedload* is the sediment moving near the bed and supported most of the time by the flow at the river bed.

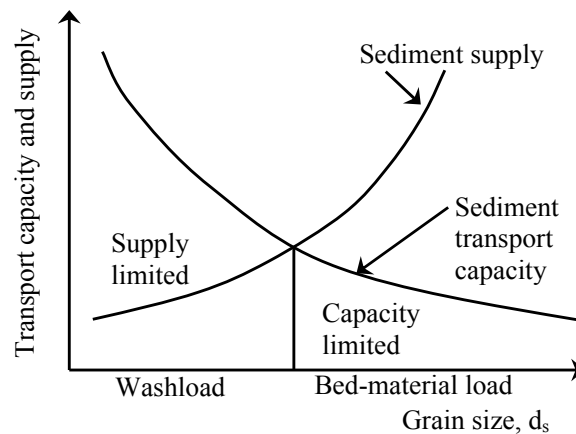


Figure 2.9: Sediment transport capacity and supply curves (Julien, 1995)

2.2.1.4. Sediment delivery ratio (SDR)

Erosion is usually expressed in tons of soils per square kilometre ($1/\text{km}^2$) or hectare e.g. ton/km^2 ; per time (year, season) e.g. tons/year ; or per storm or per day). The soils should be distinguished from sediment yield, which is the flow of sediment measured in the flowing water body in the same time period or shortly after (see Figure 2.10). Sediment delivery ratio relates the sediment yield and upland erosion (Kinnell, 2004; Novotny, 2002)

$$SDR = \frac{Y_s}{T_e} \quad (\text{eq. 2.11})$$

Where:

- Y_s = Sediment yield at a given point (e.g. catchment outlet)
 T_e = Total erosion from the upland catchment of the given point

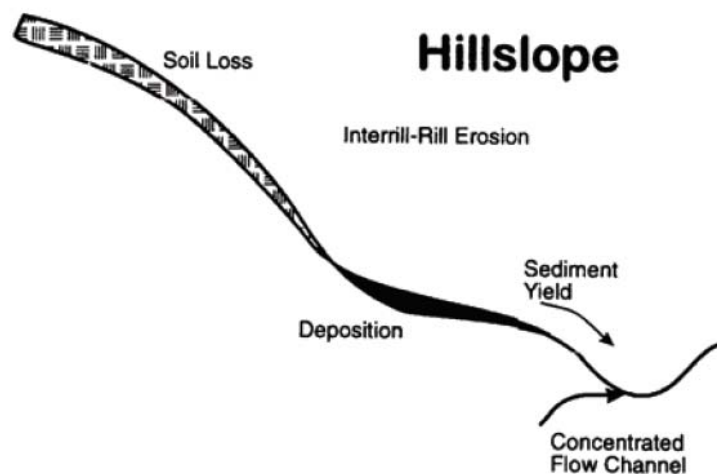


Figure 2.10: Soil erosion and deposition from a hillslope and sediment yield in the channel (Flanagan and Nearing, 1995)

2.2.2. Physical processes of soil erosion and sediment yield and prediction methods

Morgan (2005) defines “Soil erosion is a two-phase process consisting of the detachment of individual soil particles from soil mass and their transport by erosive agents such as running water and wind. When sufficient energy is no longer available to transport the particles, a third phase, deposition, occurs.” Saloranta et al (2003) state “The predominant processes that determine erosion are infiltration, run-off, detachment and transport by raindrops and overland flow (interrill erosion), detachment and transport by concentrated flow (rill erosion), and deposition”. Meyer and Wischmeier (1969, cited in Kinnell, 2004) schematically represent the processes of soil erosion by water (Figure 2.11). Therefore, in order to model soil erosion (and sediment yield) processes, the following aspects should be included: detachment capacity, transport capacity (or sediment routing) and deposition.

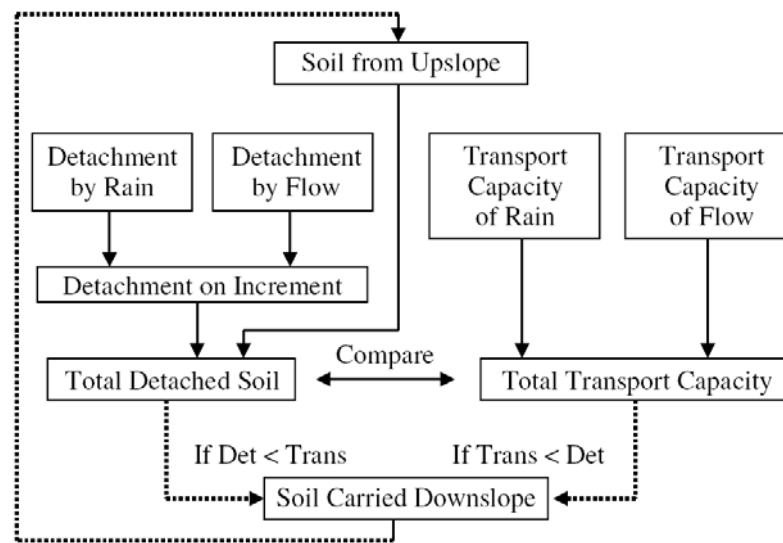


Figure 2.11: Approach used by Meyer and Wischmeier (1969) to simulate the processes of soil erosion by water (1969, cited in Kinnell, 2004)

To estimate sediment yield and upland erosion, Novotny (2002) presents the following methods:

- 1) The stream flow sampling method
- 2) The reservoir sedimentation survey method
- 3) The sediment delivery method
- 4) Bedload function methods
- 5) Method using empirical equations
- 6) Simulation catchment sediment load models

Methods 5 and 6 are used in erosion modeling at catchment scale. The *empirical equations*⁴ predict sediment yield (e.g. directly measured by method 1 or 2) by considering hydrologic factors and/or geomorphologic characteristics. Most of these empirical equations have severely limited applications, even in the region of origin (Novotny, 2002). In *catchment sediment load models (method 6)*, different physical processes are simulated. The processes can be modelled using empirical equations or process-

⁴ Discussion on empirical approach is given in section 2.6.1.2

based equations (e.g. implementing continuity equations). The models are capable of simulating individual storm events or seasonal water and sediment yields.

However, Novotny (2002) mentions: “Sediment yield measured at a catchment outlet or a point on the water course is not equal to the upland erosion. The state of the art for estimating delivery ratios has not progressed much beyond the long-established empirical relationship, and available lumped models are still inaccurate”. Above aspects should be considered carefully in implementing erosion model.

The following sections will present both empirical and physical models of soil erosion and sediment yield at catchment scale. A review of this field can be found in other works e.g. Zhang et al. (1996), Merrit et al.(2003), Aksoy and Kavvas (2005)

2.2.2.1. Empirical approach - the Universal Soil Loss Equation (USLE)

The empirical model relates to input data and the measured sediment yield based on (non-) linear regression techniques. In order to derive an empirical relation, field experiments are required comprehensively. One of the most well-known empirical equations is the Universal Soil Loss Equation (USLE) (ASAE, 2003)

The universal soil loss equation is written as

$$A = R \times K \times L \times S \times C \times P \quad (\text{eq. 2.12})$$

Where:

- A = Annual average soil loss per unit area [tons/acre/yr]
- R = Annual average erosivity of rainfall *and* runoff [(ft-tons/ac)(in/h)/yr = R-Units/yr]
- K = Soil erodibility factor [tons/ac/ R-Units]
- L = Dimensionless length factor (L=1 for standard plot)
- S = Dimensionless slope factor (S=1 for standard plot)
- C = Dimensionless cover factor (C = 1 for standard plot)
- P = Dimensionless conservation practice (P = 1 for standard plot)

Nearing et al (2001) show a major limitation of the USLE. It provides no information on non-temporal and spatial variability of erosion. In other words, the USLE explicitly predicts the long-term annual average soil loss, and it estimates spatial average of erosion on a hillslope. They (Nearing et al., 2001) also state “the critical deficiency in term of nonpoint source pollution is that the USLE predicts average soil loss only over the area of net soil loss. It does not predict deposition or sediment delivered from a field or end of a slope, nor does it provide any information on the chemical-carrying capacity or enrichment ratio of the sediment generated by erosion”. The advantages of the USLE model is that it is easy to conceptually understand and use, but it is limited in implementation outside the developed conditions (Zhang et al., 1996).

The USLE computes the annual soil loss. Some improvements on this equation have been introduced such as the Revised Universal Soil Loss Equation (RUSLE) (Renard et al., 1997), the Modified Universal Soil Loss Equation (MUSLE) (Williams and Hann, 1978). For example, the Modified Universal Soil Loss Equation (MUSLE) is used to predict soil erosion for individual events as follows:

$$Y = 11.8 \times (V \times q_p)^{0.56} \times K \times C \times P \times LS \quad (\text{eq. 2.13})$$

Where:

Y	=	Sediment yield from an individual storm in t
V	=	Storm runoff in m ³
q _p	=	The peak runoff rate in m ² /s
K	=	The soil erodibility factor
LS	=	The slope length and gradient factor
C	=	Crop management factor
P	=	The erosion-control-practice factor

The USLE approach as well as its derivatives (e.g. MULSE, RULSE) has been adopted in several catchment water quality models such as ANGPS (Young et al., 1989), SWAT (Neitsch et al., 2005). Methods used to derived parameters in the USLE is well documented in the literature (e.g. in Foster, 1982; Renard et al., 1997).

2.2.2.2. Processes-based model

A process-based (or physically-based) model in soil erosion and sediment yield prediction is a model which can express the soil erosion processes in physical senses. The mathematical algorithms inside the model can be based on the universal physical equation, e.g. mass balance or empirical relations. A review on process-based erosion model can be found in Merrit et al. (2003), or Aksoy and Kavvas (2005).

Schröder (2000) compares comprehensively three different physically-based models; namely, WEPP, EUROSEM, EROSION-2D. Schröder (2000) then investigates the detailed model algorithms of soil erosion processes including hydrological components, erosion mechanisms and sediment transport. Based on this study, the main processes in soil erosion that can be modelled as follows:

- Detachment by rain
- Detachment by flow
- Sediment deposition
- Transportation capacity of rain
- Transport capacity of flow
- Sediment routing

These processes are presented as mathematical equations in the following sections. The presentations have been mostly adopted from frequently-cited erosion models.

2.2.2.3. Detachment by rain

Morgan et al. (1998) propose that the soil detachment by raindrop impact (DR , m³/s/ m) for time step (t_s) in the EUROSEM model be calculated as:

$$DR = \frac{k}{\rho_s} KE e^{-zh} \quad (\text{eq. 2.14})$$

Where:

k	=	An index of the detachability of the soil (g/J) for which values must be obtained experimentally
ρ _s	=	Particle density (kg/m ³)

- KE = Total kinetic energy of the net rainfall at the ground surface (J/m²)
 z = An exponent varying between 0.9 and 3.1
 h = Mean depth of the surface water layer (m)

While detachment by raindrop is considered as interrill erosion in WEPP model (Foster, 1982) and is presented as:

$$D_1 = 0.0138 K_1 I^2 \quad (\text{eq. 2.15})$$

Where:

- D_1 = Detachment rate (k/m²/h)
 K_1 = An interrill erodibility parameter (kgh/Nm²)
 I = Average rainfall intensity integrated over the duration of rainfall excess (mm/h)

2.2.2.4. Detachment by flow

Morgan et al. (1998) calculate the detachment rate of soil particles by the flow (DF), including the erosion rate of the flow (E_q , m³/s/m), continually accompanied by deposition at a rate (wCv_s):

$$DF = E_q - wCv_s \quad (\text{eq. 2.16})$$

Where:

- E_q = Erosion rate of the flow (m³/s/m)
 w = Soil's rill erodibility width of flow (m)
 v_s = The particle settling velocity (m/s)
 C = Sediment concentration (m³/m³)

Nearing et al (1994; 2001) define detachment by flow as rill erosion as:

$$D_c = K_t (\tau - \tau_c) \quad (\text{eq. 2.17})$$

Where:

- D_c = Detachment capacity of clear water flow
 K_t = Soil's rill erodibility
 τ = Shear stress of flow (N/m²)
 τ_c = Soil's critical hydraulic shear strength (N/m²)

2.2.2.5. Sediment deposition

Nearing et al. (2001) define the amount of deposition as when sediment load, G , exceeds the sediment transport capacity, TC . In the WEPP model, the net deposition is computed by:

$$D_f = \frac{\beta V_f}{q} (TC - G) \quad (\text{eq. 2.18})$$

Where:

- V_f = Effective fall velocity for the sediment (m/s)
 q = Flow discharge per unit width (m²/s)
 β = A raindrop-induced turbulence coefficient (e.g. impact in rill flow, $\beta=0.5$)
 TC = Transport capacity (m³/m²/s)

In Hairsine and Rose model (Hairsine and Rose, 1992), the continuous deposition is:

$$d_i = \alpha_i v_i c_i$$

Where:

$(v_i c_i)$ = Concentration of the settling velocity class i near the bed

α = Account for non-uniform distribution of sediment concentration in the flow

2.2.2.6. Transportation capacity of rain

The transportation capacity of rain is integrated in the transportation capacity of flow since rain drops increase transport capacity of overland flow (Lal, 1990). Unfortunately, no literature was found regarding its mathematical expression.

2.2.2.7. Transport capacity of flow

Transport capacity of overland flow is the capacity of a defined runoff volume to carry a certain amount of suspended sediment.

The modified Yalin transport capacity equation is used in WEPP for rill erosion (Nearing et al., 2001):

$$T_c = k_t \tau_f^{3/2} \quad (\text{eq. 2.19})$$

Where:

T_c = Transport capacity (kg/m/s)

k_t = Sediment transport coefficient ($\text{m}^{1/2}\text{s}^2/\text{kg}^{1/2}$)

τ_f = Hydraulic shear acting on soil (N/m^2)

$$\tau_f = \rho g R s \quad (\text{eq. 2.20})$$

Where:

ρ = Fluid density (kg/m^3)

g = 9.8, Gravity constant (m/s^2)

R = Hydraulic radius (m)

s = Slope gradient (m/m)

$$k_t = \frac{T_{co}}{\tau_{so}^{3/2}} \quad (\text{eq. 2.21})$$

Where:

T_{co} = Transport capacity computed using τ_{so}

τ_{so} = Representative shear stress for entire slope

Morgan et al. (1998) define the *rill transport capacity*

$$TC = c(\omega - \omega_{cr})^\eta \quad (\text{eq. 2.22})$$

Where:

ω = Unit stream power (cm/s)

ω_{cr} = Critical value of unit stream power (= 0.4cm/s)

c, η = Experimentally derived coefficients depending on particle size

$$\omega = 10 u s \quad (\text{eq. 2.23})$$

Where:

s = Slope (%)
u = Mean flow velocity (m/s).

Interrill transport capacity:

$$TC = \frac{b}{\rho_s q} \left[(\Omega - \Omega_c)^{0.7/n} - 1 \right]^k \quad (\text{eq. 2.24})$$

Where:

k = 5
 ρ_s = The sediment density (kg/m³)
b = A function of particle size defined by:

$$b = \frac{19 - (d_{50}/30)}{10^4}$$

 Ω = Modified stream power (g^{1.5} cm^{-2/3}/s^{4.5})
 d_{50} = Median grain sizes from silt to coarse sand

2.2.2.8. Overland sediment routing

The sediment routing is physically based on the sediment continuity equation, which addresses soil erosion using differential mass balance equations for describing sediment continuity on a land surface. The fundamental equation for mass balance of sediment in a single direction on a hillslope profile is given as (Nearing et al., 2001):

$$\frac{\partial(cq)}{\partial x} + \frac{\partial(ch)}{\partial t} + S = 0 \quad (\text{eq. 2.25})$$

Where:

c = Sediment concentration (kg/m³)
q = Unit discharge of runoff (m²/s)
h = Depth of flow (m)
x = Distance in the direction of flow (m)
S = Source/sink term for sediment generation (kg/m²/s)

For the case of steady-state conditions, and incorporating the concepts of rill and interrill erosion, the above equation can be rewritten in the WEEP model as (Foster et al., 1995):

$$\frac{dG}{dx} = D_r + D_i \quad (\text{eq. 2.26})$$

Where:

G = Sediment load per unit width in the flow (kg/m/s) (equal to cq , eq. 2.25)
 D_r = Net rill erosion rate per unit area of rill bottom
 D_i = Interrill sediment delivery to the rill (as with rill erosion, expressed on a per unit rill area basis)

Morgan et al. (1998) route sediment along the flow path in the EUROSEM model based on a numerical solution of the dynamic mass balance equation:

$$\frac{\partial(AC)}{\partial t} + \frac{\partial(QC)}{\partial x} - e(x, t) = q_s(x, t) \quad (\text{eq. 2.27})$$

Where:

C	=	Sediment concentration (m ³ /m ³)
A	=	Cross-sectional area of the flow (m ²)
Q	=	Discharge (m ³ /s)
q _s	=	External input or extraction of sediment per unit length of flow (m ³ /s/m)
e	=	Net detachment rate or rate of erosion of the bed per unit length of flow (m ³ /s/m)
x	=	Horizontal distance (m)
t	=	Time (s)

For channel flow q_s represents lateral inflows of sediment from the base of adjacent hillsides. When applied to overland flow over hillslopes, q_s becomes zero.

Hairsine and Rose (1992) define the mass balance equation as:

$$\frac{\partial(c_i q)}{\partial x} + \frac{\partial(c_i h)}{\partial t} = e_i + e_{di} + r_i + r_{ri} - d_i \quad (\text{eq. 2.28})$$

Where:

e _i , e _{di}	=	Entrainment by rainfall, re-entrainment by rainfall, respectively
r _i , r _{ri}	=	Entrainment by surface water flow, re-entrainment by surface water flow
d _i	=	Continuous deposition term
i	=	Subscript indicates the particle settling velocity class of the sediment

Borah (1989) describes the sediment continuity equation for overland flow elements in the RUNOFF model in dynamic form and is written as:

$$\frac{\partial(Q_s)}{\partial x} + \frac{\partial(CA)}{\partial t} = q_s + g \quad (\text{eq. 2.29})$$

Where:

Q _s	=	Volumetric sediment discharge (m ³ /s)
C	=	The volumetric concentration of sediment (m ³ /m ³)
A	=	Cross sectional area of flow (m ²)
q _s	=	Volumetric rate of lateral sediment inflow per unit length (m ³ /s/m)
g	=	Net volumetric rate of material exchange with the bed per unit length (m ³ /s/m)

2.2.2.9. Sediment composition

Composition of particle classes is important for estimating contaminant load on sediment since different contaminants may have different behaviours depending on sediment sizes. Contaminant concentration on the clay particles is highest adsorbed and is travelled as washload, while contaminant in coarse sediment may be deposited or travelled as bedload (as shown in Figure 2.9). Clay which has the highest absorption of contaminant travels as washload, while coarse sediment and associated contaminants may be deposited and/or can travel as bedload. Foster et al. (1995) propose a scheme based on extensive experimentation in order to estimate 5 sediment compositions (as illustrated in Table 2.2).

Table 2.2: Distribution of detached particle sizes and their densities (Foster et al., 1995; Hartley, 1987a)

Particle type	Size (mm)	Specific gravity	Fraction in detached sediment
Primary clay	0.002	2.65	$F_{cl} = 0.26 O_{cl}$
Primary silt	0.01	2.65	$F_{si} = O_{si} - F_{sg}$
Small aggregate	0.03 ^[1]	1.80	$F_{sg} = 1.8 O_{cl}$ ^[6]
	0.2 ($O_{cl} - 0.25$) + 0.03 ^[2]		$F_{sg} = 0.45 - 0.6 (O_{cl} - 0.25)$ ^[7]
	0.1 ^[3]		$F_{sg} = 0.6 O_{cl}$ ^[8]
Large aggregate	0.3 ^[4]	1.60	$F_{lg} = 1 - F_{cl} - F_{si} - F_{sg} - F_{sa}$
	2 O_{cl} ^[5]		
Primary sand	0.2	2.65	$F_{sa} = O_{sa} (1 - O_{cl})^5$

^[1] $O_{cl} < 0.25$; ^[2] $0.25 \leq O_{cl} \leq 0.60$; ^[3] $O_{cl} > 0.60$; ^[4] $O_{cl} \leq 0.15$; ^[5] $O_{cl} > 0.15$; ^[6] $O_{cl} \leq 0.25$;

^[7] $0.25 \leq O_{cl} \leq 0.50$; ^[8] $O_{cl} > 0.5$

Where:

O_{cl} = Clay fraction in matrix soil

F_{cl} = Fraction of the sediment composed of the primary clay class

O_{si} = Silt fraction in matrix soil

F_{si} = Fraction of primary silt class in the sediment

F_{sg} = Fraction of small aggregate

F_{lg} = Fraction of the large aggregate in the sediment

F_{sa} = Fraction of primary sand class

2.3. Nitrogen transports and transformations

Although nitrogen is very essential for the development of plants and animals, it may be harmful for aquatic systems and human beings (Hatch et al., 2002). Nitrogen, in addition to phosphorus, is a limiting factor of eutrophication which is a severe problem for ecosystems. Nitrate nitrogen (NO_3) in drinking water causes serious diseases in human, like stomach cancer (Hatch et al., 2002; Heathwaite et al., 1993). Recognizing this hazardous aspect, the World Health Organization, as well as many countries has measured concentration of nitrogen in different forms as shown in Table 2.3. In addition, efforts to reduce nitrogen in water have been carried out, e.g. European Nitrate Directive (Heathwaite et al., 1993), European Water Directive (Blösch, 2001), The Total Maximum Daily Load (NRC, 2001).

Table 2.3: Guide and maximum admissible concentration of various forms of nitrogen (N) in portable water (ECE, 1993) (Hatch et al., 2002)

Country/organization	Form of nitrogen	Guide (mg l ⁻¹)	Maximum admissible concentration (mg l ⁻¹)
European Community	Nitrate	25.0	50.0
	Nitrite	—	0.1
	Ammonium	0.05	0.5
USA	Nitrate	—	45.0 ^a
World Health Organization	Nitrate	—	45.0 ^a

^a Limit defined as 10 mg N l⁻¹; recalculated to mg NO_3^- l⁻¹ = 44.3, rounded up to 45.

This section first presents a brief introduction about nitrogen sources and its popular forms. The introduction is followed by descriptions of nitrogen transformation processes in soil and water. The nitrogen transports in catchment is emphasized in the next part. Finally, nitrogen loss within a catchment will be presented.

2.3.1. Nitrogen sources

Nitrogen comes, basically, from 2 sources: (1) natural sources, and (2) anthropogenic sources. The natural sources are those existing in the soil and water as well as the wet and dry atmospheric deposition. Fuel combustion from human can also contribute to the atmospheric deposition (Benbi and Richter, 2003; Hatch et al., 2002; Wayne, 1993). Among the human-induced sources (e.g. agricultural activities, wastewater discharge, runoff), fertilizers including inorganic fertilizers, organic compounds as animal waste, manure, sludge etc. are considered as the greatest contributors of nitrogen to the environment (Ritter and Bergstrom, 2001).

2.3.2. Nitrogen forms

Nitrogen exists in the environment⁵ in inorganic and organic forms. The inorganic forms compose of Ammonia (NH_3), ammonium (NH_4), nitrite (NO_2), and nitrate (NO_3) while most of the organic forms are in compounds of amino acids. These different forms of nitrogen are inter-related as shown in Figure 2.12. Nitrogen cycle can also be found on a global scale (Jarvis, 1999), farm scale (Hatch et al., 2002) or aquatic system (Heathwaite, 1993). The farm nitrogen cycle is illustrated here since it is the most relevant to nitrogen transport and transformation at catchment scale.

2.3.3. Nitrogen transformations

As can be seen in Figure 2.12, the nitrogen cycle includes a number of transformation processes as follows: ammonification (mineralization) and immobilization; nitrification and denitrification; plant uptake; and volatilization. Detailed descriptions of these processes can be found in a number of materials (Hatch et al., 2002; Heathwaite, 1993; Novotny, 2002; Söderlund and Svensson, 1976) as a summary in Shukla (2000). The following sections present a number of important aspects of these processes which are also summarized in Table 2.4.

⁵ Limited here as soil and aquatic environment

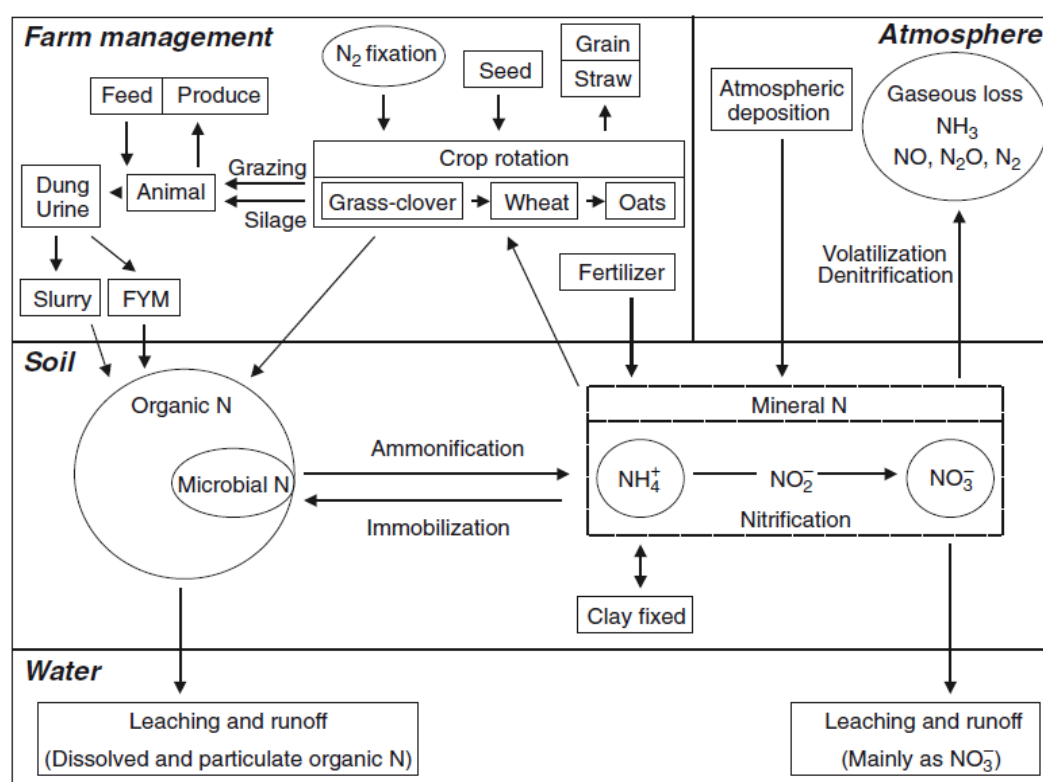


Figure 2.12: A simplified diagram of the farm nitrogen cycle (Hatch et al., 2002)

Table 2.4: Key processes in controlling N dynamics (Jarvis, 1999)

Process	Outcome	Major controlling factors
Uptake into biomass and assimilation	Removal of mobile, mineral N from soil available pools	<ul style="list-style-type: none"> • Environmental (H_2O and temperature) • Carbon fixation • Soil type and conditions • Biomass community structure and population
Mineralization /immobilization	Release/removal of mobile mineral N into available pools	<ul style="list-style-type: none"> • Soil type and conditions (temperature and H_2O) • Organic matter/residue quality/quantity • System stability and equilibrium
Nitrification	Transfer from relatively immobile (NH_4^+) to highly mobile (NO_3^-) form (some release of N_2O and NO_x)	<ul style="list-style-type: none"> • Substrate (NH_4^+) concentration • Soil aerobicity (and other environmental conditions) • Nitrifying populations • Other soil (e.g. pH) conditions
Volatilization	Transfer from terrestrial state to short-lived atmospheric forms (NH_3 and particulate NH_4^+)	<ul style="list-style-type: none"> • Substrate [$\text{NH}_4^+/\text{NH}_3$ (dissolved)] concentration • Soil pH • Environmental conditions (including windspeed)

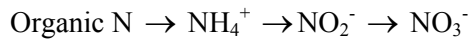
Process	Outcome	Major controlling factors
Denitrification	Transfer from terrestrial and aquatic states to atmosphere [N ₂ O(NO _x) and N ₂]	<ul style="list-style-type: none"> • Enzymic activities • Substrate (NO₃⁻) concentration • Anoxia • Environmental condition (temperature) • Energy source
'Leaching'	Trasfer of mobile NO ₃ ⁻ (also NO ₂ ⁻ , dissolved organic forms and some NH ₄ ⁺) from terrestrial to aquatic system	<ul style="list-style-type: none"> • NO₃⁻ concentration • Hydrological pathways • Soil type/conditions • Others N cycling processes

2.3.3.1. Mineralization (ammonification) and immobilization

Nitrogen mineralization is the process where the organic forms of nitrogen are converted into ammonium nitrogen (NH₄-N). This process is mainly carried out by microorganisms (Ritter and Bergstrom, 2001). In contrast to mineralization, immobilization is the biological assimilation of inorganic of nitrogen by plants and microorganisms to form organic compounds. Immobilization and mineralization occur simultaneously in the soil.

2.3.3.2. Nitrification

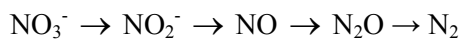
Nitrification is the microbial oxidation of ammonium-N (NH₄⁺) produced from mineralization to nitrite (NO₂⁻) and further to nitrate (NO₃⁻). The nitrification process proceeds as follows:



The last reaction, that is the conversion of NO₂⁻ to NO₃⁻, is faster than the conversion of NH₄⁺ to NO₂⁻. Consequently, very little nitrite accumulates in soils and sediment (Novotny, 2002).

2.3.3.3. Denitrification

Under anaerobic conditions, denitrification process will remove excess NO₃⁻ from soil and return N₂ to the atmosphere. Biological denitrification proceeds as:



The biochemistry of denitrification is complicated and poorly understood, however, the environmental factors affecting denitrification are relatively well known (Novotny, 2002).

2.3.3.4. Nitrogen fixation

Biological nitrogen fixation is a process by which soil microorganisms, in symbiosis with leguminous plants, use atmospheric nitrogen and change it to an organic form.

2.3.3.5. Volatilization

Ammonia volatilization occurs at high soil or water pH values (i.e. acidic water, soil). It is a process where the ammonium ion (NH₄⁺) is converted to gaseous ammonia (NH₃), which volatilizes to the atmosphere as a loss.

2.3.3.6. N uptake and assimilation

Nitrogen uptake or assimilation by plants and animals is the most important fraction of the total N input for living systems. The available nitrogen includes nitrate and ammonium, which is in equilibrium with organic nitrogen (Follett, 1995).

2.3.4. Nitrogen transport (pathways) in catchment

Nitrogen transport in or out of catchment can be seen as the nitrogen loss from the catchment. The main paths include:

- Leaching of nitrate.
- Loss of nitrogen in gaseous forms because of volatilization and denitrification.

Dissolved nitrogen (e.g. nitrate), and particulate nitrogen (e.g. ammonium, organic nitrogen) which is adsorbed to sediment, are transported by runoff. Ghadiri and Rose (1992) mention “with the exception of nitrogen in nitrate form, or converted to gaseous form, the loss of nitrogen is chiefly associated with the loss of sediment”

Figure 2.13 shows the pathway of nitrogen transport from hillslopes to stream. The transport mechanism involves a number of aspects, for example: soil structure and type; rainfall; the amount of nitrate supplied in fertilizers, plant cover and root activities. Consequently, the amount and form of nitrogen transported vary from different land uses (Heathwaite et al., 1993).

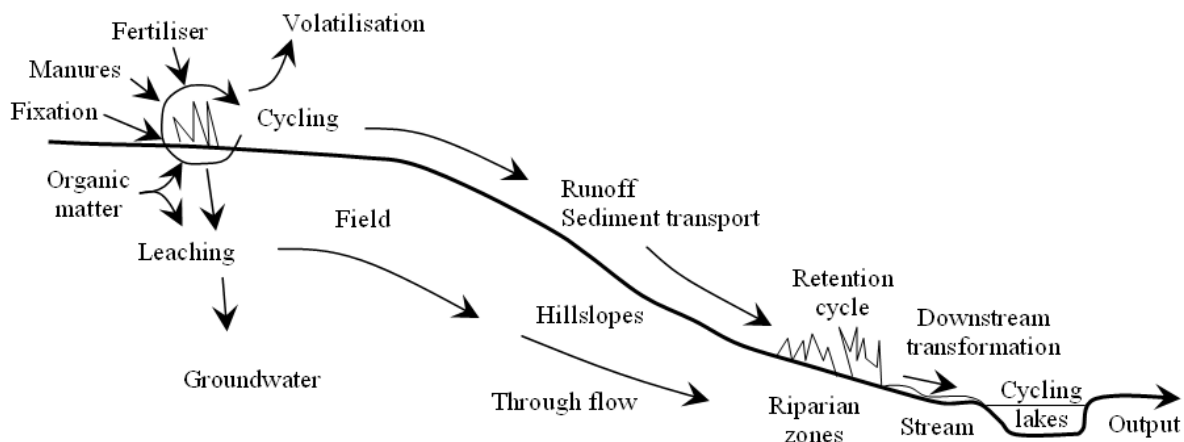


Figure 2.13: The pathway of nitrogen delivery from hillslopes to stream (Heathwaite et al., 1993)

Nitrogen leaching below the root zone is mainly nitrate which is transported to groundwater. This process involves a number of factors, e.g. amount of available nitrogen, mass of infiltrating water and hydraulic conductivity of the material, water table depth, and denitrification potential. Together with runoff mechanisms, leaching is a primary flow path of nitrogen loss. Heathwaite et al. (1993) mentions that inorganic nitrogen is the dominant nitrogen species in runoff from arable land, whereas organic nitrogen and ammonium-nitrogen are the major nitrogen species in grassland runoff. They (Heathwaite et al., 1993) also concludes that leaching is the main process of nitrogen transfer from hillslopes to stream.

Nitrogen loss due to soil erosion is also a source of concern. Erosion losses of total nitrogen from agricultural lands may vary from 1 to 100 kg N/Ha/year (Benbi and Richter, 2003). Rose and Dalal

(1988, cited in Benbi and Richter, 2003) mention that “more than 90% nitrogen loss in eroded sediment is organic matter”. The concentration of nitrogen in sediment is usually higher in soil, which declines when the sediment yield increases (Rose and Dalal, 1988, cited in Benbi and Richter, 2003). Ritter and Bergstrom (2003) report that the riparian zones reduces the nitrogen transported to the aquatic system. The riparian removes nitrogen by plant uptake, denitrification and sediment trapping. Ritter and Bergstrom (2001) state the plant uptake will reduce its efficiency of removing nitrogen if the plants are not harvested.

2.3.5. Nitrogen modeling at catchment scale

Nitrogen modeling at catchment scale requires an understanding of nitrogen sources, forms, transformation as well as nitrogen transports. Detailed simulation of each process is rather complicated. Thus, attempts to model nitrogen dynamics within a catchment are limited by simplifications. Basically, these processes are considered as follows: (1) nitrogen input sources (e.g. atmospheric deposition, fertilizer), (2) nitrogen transformation (e.g. immobilization, nitrification), (3) nitrogen losses (e.g. leaching, runoff and erosion, ammonia volatilization, plant uptake) (Benbi and Richter, 2003).

While the nitrogen sources are assumed as input data for models, the other two components can be expressed in mathematical algorithms and then implemented in models.

2.3.5.1. Nitrogen transformations

Nitrogen transformation is often modelled by a simple approach according to the first-order kinetics. For example, *nitrogen mineralization* can be modelled as:

$$\frac{dN}{dt} = -kN \quad (\text{eq. 2.30})$$

Where:

N = Concentration of mineralizable substrate

t = Time

k = Rate of mineralization

This equation is integrated between time t and t_0 :

$$N_t = N_o e^{-kt} \quad (\text{eq. 2.31})$$

Where:

N_o = Initial substrate concentration

N_t = Substrate concentration at time t

2.3.5.2. Nitrogen losses

Denitrification losses can be modelled by taking into account the relationship between the denitrification rate with nitrate, water extractable organic carbon, soil water saturation and temperature, e.g. proposed by Rolston (1984, cited in Benbi and Richter, 2003) as follows:

$$\frac{dG}{dt} = k_1 \theta_w f_a C_w N \quad (\text{eq. 2.32})$$

Where:

$$\frac{dG}{dt} = \text{Denitrification rate}$$

- N = Nitrate concentration
 C_w = Water extractable organic carbon
 θ = Soil water saturation
 k₁ = Denitrification rate coefficient
 f_w and f_a = Empirical functions to account for water content and temperature effects

In LEACHN model (Hutson and Wagenet, 1991), denitrification is modelled using Michaelis-Menten kinetics:

$$\frac{dN_{NO_3}}{dt} = \frac{k_{denit} N_{NO_3}}{(N_{NO_3} + c_{sat})} \quad (\text{eq. 2.33})$$

Where:

- k_{denit} = Potential rate
 c_{sat} = Haft-saturation constant

Ammonia volatilization is considered along with situation-specific processes. Benbi and Richter (2003) list a number of formulas which are applied in different areas such as ammonia (NH₃) volatilization from soil and surface manure, urea; ammonia volatilization from folded soil. In LEACHN model, volatilization follows a first-order process (Hutson and Wagenet, 1991):

$$\frac{dN_{NH_4}}{dt} = -k_{volat} N_{NH_4} \quad (\text{eq. 2.34})$$

Nitrate leaching is simulated either by a deterministic or a stochastic approach as further discussed in section 2.6.1, “model classification.” The Richard equation for water flow in unsaturated zone coupled with the convection-dispersion equation for chemical transport is a typical deterministic approach, while transfer function model are regarded as a stochastic model (Addiscott and Wagenet, 1985; Benbi and Richter, 2003; Stockdale, 1999).

The Richard equation:

$$\frac{d\theta}{dt} = \frac{\partial}{\partial z} \left[K(\theta) \frac{\partial H}{\partial z} \right] - A(z, h) \quad (\text{eq. 2.35})$$

Where:

- θ = Volume water content (m³/m³)
 K(θ) = Water content-dependent hydraulic conductivity (mm/day)
 $\frac{\partial H}{\partial z}$ = Hydraulic gradient (mm/mm)
 A = Extraction of water by root (1/day)
 z = Depth (mm)
 t = Time (days)

Convection-dispersion equation, for absorbing, degrading chemical in LEACHN model

$$\frac{\partial(\theta c)}{\partial z} + \frac{\partial(\rho s)}{\partial t} = \frac{\partial}{\partial z} \left[\theta D(\theta, q) \frac{\partial c}{\partial z} - qc \right] - U(z, t) \pm \phi(z, t) \quad (\text{eq. 2.36})$$

Where:

- c = Chemical concentration in the liquid phase (mg/dm³)
 s = Chemical concentration in absorbed phase (mg per kg dry soil)
 $D(\theta, q)$ = Effective dispersion coefficient - function of water content and pore water velocity (mm²/day)
 ρ = Soil bulk density (kg/dm³)
 q = Water fluid density (mm/day)
 $U(z, t)$ = Plant uptake of nitrogen (mg/dm³/day)

The absorbed and solution phase concentration are related by the linear isotherm:

$$s = K_d c \quad (\text{eq. 2.37})$$

Where:

$$K_d = \text{Participation or distribution coefficient (dm}^3/\text{kg)}$$

The transfer function model is also very popular in modeling nitrate leaching. A review of this type of model can be found in Addiscott and Wagenet (1985), Benbi and Richter (2003), Stockdale (1999). This approach estimates the probability density function of travel times of solute at different soil depths, based on monitoring data. Jury (1982, cited in Addiscott and Wagenet, 1985; Jury and Horton, 2004, chapter 7) proposes the distribution function as follow:

$$P_L(I) = \int_0^1 f_L(I) dI \quad (\text{eq. 2.38})$$

Where:

$$f_L(I) = \text{Travel time probability density function summarizing the probability (P}_L\text{) that a solute added at the soil surface will arrive at depth L as the quantity of water applied at the surface increases from I to (I + dI)}$$

Nitrogen loss by runoff

a) Dissolved nitrogen

Dissolved nitrogen such as nitrate and ammonium can be modelled in either an empirical or a physical sense. Loading function is most often seen in model codes for dissolved contaminants. In CREAMS/GLEAMS model (Knisel et al., 1993; Knisel and Walter, 1980), dissolved contaminant is calculated as:

$$C_{ro} = 0.1CQ \quad (\text{eq. 2.39})$$

Where:

$$\begin{aligned}
 C_{ro} &= \text{Dissolved contaminant (concentration of nitrate or ammonium) in runoff (kg/ha)} \\
 C &= \text{Concentration of phosphate in water layer 1 (mg/l)} \\
 Q &= \text{Runoff (cm)}
 \end{aligned}$$

Based on the conservation of mass principle, Borah et al (2002) proposes a method to calculate dissolved contaminants in runoff in the form of a continuity equation:

$$\frac{\partial(VC_r)}{\partial X} + \frac{\partial C_r}{\partial T} = q_e \quad (\text{eq. 2.40})$$

Where:

- b = Average velocity of runoff water (cm/s)
 C_r = Chemical mass load in runoff ($\mu\text{g}/\text{cm}^2$)
 q_e = Chemical mass entrainment from mixing soil layer to surface runoff during time ($\mu\text{g}/\text{cm}^2/\text{s}$)
 X = Down slope position (cm)
 T = Time (s)

b) Particulate nitrogen

Ammonium and organic nitrogen can be absorbed in soil, and transported in eroded sediment by runoff. Thus, the concentration of the absorbed contaminant is a function of sediment yield and enrichment ratio (ER), which is defined as the ratio of runoff sediment content to surface soil content before runoff (Sharpley, 1995). The loading function is used in many catchment water quality models such as SWAT (Arnold et al., 1994), EPIC (Williams, 1995):

$$C_{\text{sed}} = 0.001(\text{SY})(\text{ER})C \quad (\text{eq. 2.41})$$

Where:

- C_{sed} = Concentration of ammonium or organic nitrogen loss in eroded sediment (kg/ha)
 SY = Sediment yield (ton/ha)
 ER = Enrichment ratio
 C = Concentration of ammonium or organic nitrogen in top soil layer (g/ton)

Borah et al (2002) also develop a continuity equation for absorbed nutrients as follows:

$$\frac{\partial(VC_s)}{\partial X} + \frac{\partial C_s}{\partial T} = q_s \quad (\text{eq. 2.42})$$

Where:

- V = Average velocity of runoff water (cm/s)
 C_s = Chemical mass load adsorbed with sediment ($\mu\text{g}/\text{cm}^2$)
 q_s = Chemical mass exchange rate (source/sink) with sediment ($\mu\text{g}/\text{cm}^2/\text{s}$)
 X = Down slope position (cm)
 T = Time (s)

2.4. Phosphorus transports and transformations

Similar to other nutrients (e.g. nitrogen), phosphorus is an essential element for plant and animal growth and production. However, excess phosphorus in agriculture is transported into the aquatic system, and consequently causes a problem of eutrophication. A typical example is the Chesapeake Bay (Sharpley, 2000), where the role of phosphorus in causing eutrophication was comprehensively reported. Eutrophication can lead to decreasing of ecosystem diversity since the presence of too many algae will inhibit the living conditions of other species. In addition, taste and odour caused by algae also affect people lives when present in drinking water sources, and recreational areas. It should be noted that, although nitrogen, carbon, and phosphorus all are associated with accelerated eutrophication, researchers focus the most on phosphorus since it is very difficult to control the exchange of nitrogen and carbon between the atmosphere and water body and the fixation of atmospheric nitrogen by blue-green algae (Sharpley et al., 1996; Sharpley and Smith, 1990).

A study of phosphorus dynamics at catchment scale requires knowledge on several factors. For instance, (1) what phosphorus sources, forms and transformation are in soil and water? and (2) how is phosphorus transported within a catchment? Section 2.1 and 2.2 will focus on these two questions. Subsequently, phosphorus modeling approaches are reported.

2.4.1. Phosphorus sources

Campbell and Edwards (2001) and Haygarth and Macleod (2003) mention that phosphorus can come from different sources, e.g. rainfall, plant residues, commercial fertilizers, animal manures, municipal agriculture, and industrial waste. In addition, the natural weathering processes of soil mineral also contributes to phosphorus sources (e.g. described in Filippelli, 2008). Among these, agricultural runoff (surface and subsurface) and erosion in phosphorus-excess areas are of serious concern (Filippelli, 2008).

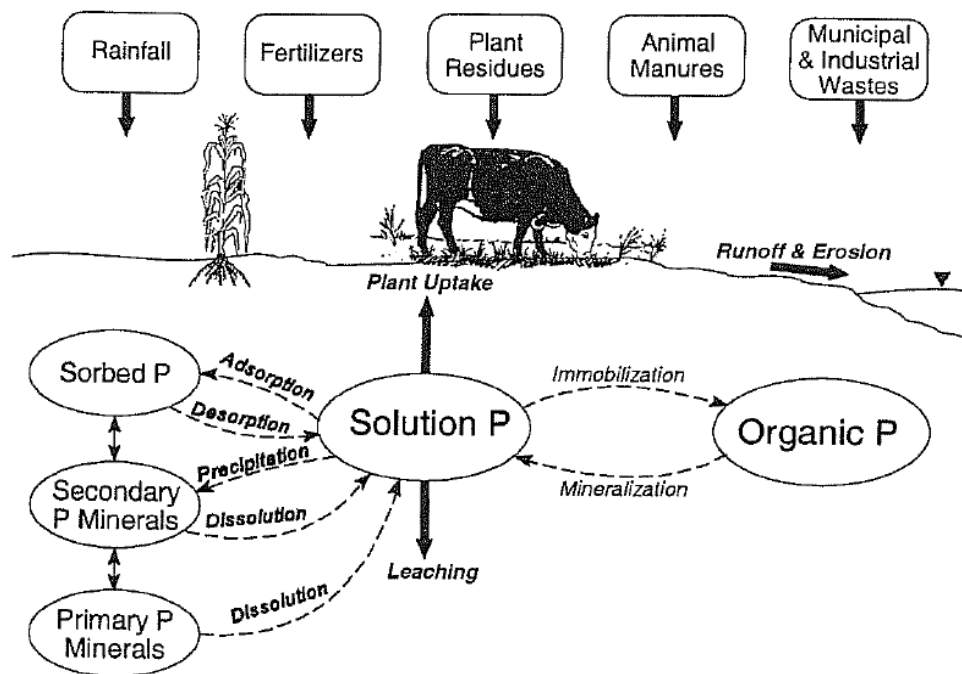


Figure 2.14: A representation of the phosphorus cycle in the soil-water-animal-plant system (Campbell and Edwards, 2001)

Phosphorus exists in different forms in soil and water. Globally, it is usually described within a phosphorus cycle. The cycle includes interactions, transformations and transports happening through different processes, e.g. physical, chemical and biological processes (Campbell and Edwards, 2001; Filippelli, 2008; Leinweber et al., 2002; Sharpley, 2007; Sharpley et al., 2003). Figure 2.14 is an example of a phosphorus cycle in a soil-water-animal-plan system. The soil-water- animal-plan system is adopted here since it is relevant to the understanding of how phosphorus is generated, transformed and transported at catchment scale. The next section will present various forms of phosphorus in soil and water, and an explanation of how it is transformed and finally transported to an aquatic environment, e.g. rivers.

2.4.2. P forms

According to the current classification in the field, three groupings are used in order to classify phosphorus, although they are inter-related. These groupings are as follows:

- Inorganic and organic
- Reactive and unreactive
- Soluble/dissolved and particulate

Organic versus inorganic (chemical aspect)

According to Leinweber et al. (2002) and Sharpley et al. (1996) inorganic phosphorus in combination with aluminium, iron, and calcium compounds are available to plant. Meanwhile, organic phosphorus consists of under-composed residues, microbes, and organic matter. Leinweber et al. (2002) mention that the most important organic compound in most soils is phytic acid, which can form up to 80% of the organic. Soil organic availability to plants and water sources is still poorly understood (Leinweber et al., 2002).

Reactive versus unreactive phosphorus (analytical aspect)

Since the common analytical method can not perfectly distinguish soluble organic phosphorus and soluble inorganic phosphorus in water, it is useful to introduce the reactive and unreactive terms (Boyd, 2000, p.202) commonly used in analytical routines in laboratory.

Particulate versus dissolved phosphorus (process/modeling aspect)

The particulate and dissolved or soluble phosphorus term is found very useful when describing transported phosphorus associated with water and sediment. These terms relate to the size fractions of phosphorus. While the particulate phosphorus is defined as phosphorus associated with particles $>0.45 \mu m$, the dissolved phosphorus is the fraction below this threshold. These two fractions are determined using filters with appropriate sizes. Lazzarotto (2004) mentions that the dissolved P [phosphorous] is often the dominant form in surface runoff or preferential flow and is directly available for algae. Therefore, it is of special concern for the eutrophication of surface waters. The particulate and dissolved terms can be used together with the first two terms (organic vs. inorganic and reactive vs. unreactive phosphorus). Figure 2.15 shows the inter-relations between the reactive and unreactive terms and the size fractionation which are also used as the dissolved and particulate terms.

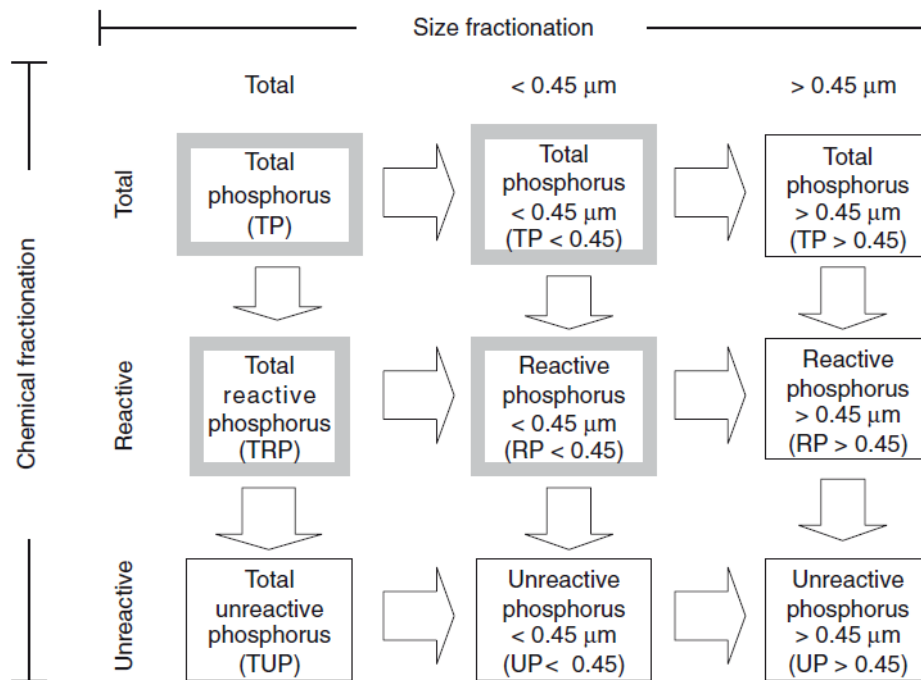


Figure 2.15: Operational defined phosphorus fractions determined in water, showing directly determined fractions (in boxes with shaded borders) and fractions determined by difference (Leinweber et al., 2002)

Haygarth and Sharpley (2000) find that it is confusing with the various phosphorus forms described in the community by experts ranging from hydrologist, chemist to soil experts. They propose a classification frame for describing phosphorus forms as shown in Table 2.5. It still needs to be further refined for practical use (Haygarth and Sharpley, 2000).

Table 2.5: Suggested methodologically defined classification of phosphorous forms in water with their equivalent established terms (Haygarth and Sharpley, 2000)

New classification	Equivalent “established” term ^(*)
RP (< 0.45)	Molybdate-reactive P (MRP), dissolved-reactive P (DRP), solute-reactive P (SRP) dissolved molybdate-reactive P, orthophosphate, inorganic P, phosphate
RP (unf)	Total reactive P (TRP), raw unfiltered sample
TP (< 0.45)	Total dissolved P (TRP)
TP (unf)	Total P on a raw unfiltered sample (TP)
UP (< 0.45)	Dissolved organic P (DOP), soluble organic P (SOP), dissolved nonreactive P (DNRP)
TP (> 0.45)	Particulate P (PP)
RP (> 0.45)	Molybdate-reactive particulate P (MRPP), particulate-reactive P

^(*)May not necessarily be correct.

2.4.3. Phosphorus transformations in soil

As discussed in the previous section, phosphorus exists in different forms. In this section, the links among these forms are introduced. There are some typical phosphorus transformation processes as observed in Figure 2.14. The absorbed and desorbed processes link the dissolved phosphorus to the

particulate forms. The mineralization and immobilization processes convert the organic forms to the soluble forms. Other transformation processes are not often observed in modeling nutrient dynamics at catchment scale though they are considered at field scale models. Thus, the following sections will focus only on the typical processes

2.4.3.1. Mineralization and immobilization

Generally, mineralization and immobilization are opposing-processes. While organic phosphorus is converted to mineral phosphorus in mineralization, the conversion of mineral phosphorus to microbial biomass is found in immobilization. These two processes occur continuously and simultaneously (Campbell and Edwards, 2001).

2.4.3.2. Adsorption and desorption

Similar to mineralization and immobilization, adsorption and desorption are opposing-processes. Constituents exist in soil if they are adsorbed to the soil; otherwise, they exist in solution. Relationships between adsorbed and desorbed phosphorus concentrations are commonly specified in the forms of isotherms, which relate adsorbed phosphorus concentration to equilibrium solution phosphorus concentration (McGechan and Lewis, 2002).

2.4.3.3. Precipitation versus dissolution

Precipitation or dissolution is often treated not as a separate set of opposing processes, but is instead considered part of the adsorption or desorption processes (McGechan and Lewis, 2002).

2.4.3.4. Plant uptake

Crop uptake affects pollution by phosphorus. However, the effect is not as clear or immediate as adsorption or desorption and precipitation or dissolution. Plants primarily use inorganic phosphorus extracted from the soil solution, thus decrease soil solution phosphorus concentration. Phosphorus uptake is controlled by plant demand or by its ability to get phosphorus from soil (Jones et al., 1984). Some typical phosphorus uptake rates are shown in Table 2.6.

Table 2.6: Typical P uptake in common crops (Campbell and Edwards, 2001)

Crop	Yield (kg/ha)	P uptake (kg/ha)
Corn	11,300	50
Soybeans	3,460	26
Grain sorghum	8,400	39
Wheat	9,500	25
Oats	3,600	20
Barley	6,500	32
Tall fescue	13,500	55
Clover	13,500	44
Bermudagrass	18,000	47
Alfalfa	18,000	59

2.4.4. Phosphorus transport (pathways) in catchment

Phosphorus transport at catchment scale is classified into two groups. Soluble or dissolved phosphorus is transported together with runoff or leaching. Particulate or sediment – associated phosphorus is transported with eroded materials. In this thesis, the soluble phosphorus is considered as pure phosphate phosphorus (P-PO₄), and particulate phosphorus includes phosphate phosphorus and organic phosphorus. During transportation, reaction or exchange between different phosphorus forms can occur as illustrated in Figure 2.16.

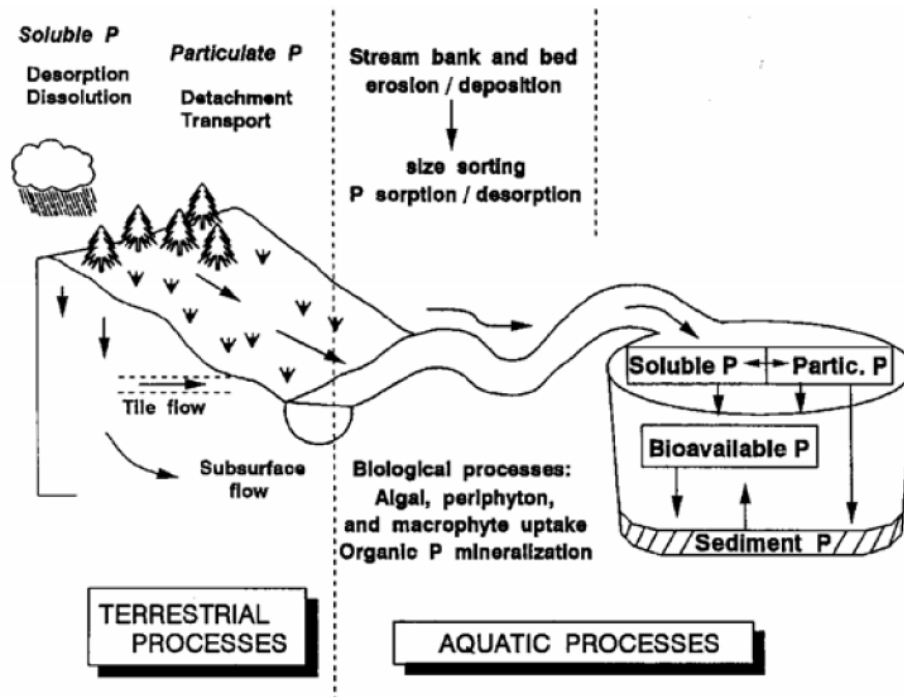


Figure 2.16: Processes of the transfer of P from terrestrial to aquatic ecosystems (Sharpley et al., 1996)

2.4.5. Modeling phosphorus at catchment scale

The modeling of phosphorus at catchment scale comprises of phosphorus transformation and phosphorus transportation. Modeling phosphorus transformation is given by the method for adsorption and desorption, other transformation processes are usually described by the first-order equation as presented in section “nitrogen.”

2.4.5.1. Adsorption and desorption

Standard equations have been used to describe the relationship between adsorbed and solution phosphorus, referred to as Langmuir and Freundlich isotherm equation. See McGeachan and Lewis (2002) for a review of other approaches . The Langmuir equation is given by:

$$C_A = \frac{Q^o b C_s}{1 + C_s} \quad (\text{eq. 2.43})$$

Where:

- C_A = Adsorbed phosphorus concentration
- C_s = Solution phosphorus concentration

- Q^0 = Maximum adsorption at the given temperature
 b = A parameter related to adsorption energy

If the adsorption energy is not constant, the isotherm might be better described by the Freundlich isotherm equation, given by:

$$C_A = KC_S^{1/n} \quad (\text{eq. 2.44})$$

Where K, n are constants.

Sharpley and Smith (1989, cited in Bnayahu Bar-Yosef, 2003) assume that the soluble phosphorus(SP) concentration of runoff can be predicted from the rate of phosphorus desorption and the effective depth of the soil layer in which surface soil and runoff interact:

$$P_r = \frac{K_{pr} \times P_s \times E \times \rho \times t^\alpha \times W_p^\beta}{V_p} \quad (\text{eq. 2.45})$$

Where:

- P_r = Average soluble phosphorus concentration in runoff for an individual event (mg/l)
 P_s = Extractable phosphorus content of surface soil, 0-55mm before each runoff event (mg/kg)
 E = Effective soil depth (mm)
 ρ = Bulk density of soil (kg/l)
 t = Runoff event duration (min)
 W_p = Runoff water/soil (suspended sediment) ratio
 V_p = Total runoff during the event (mm)
 K_{pr}, α, β = Constants for a given soil, 0.05-0.54, 0.12-0.17, 0.3-0.62, respectively.

2.4.5.2. Phosphorus transportation

Similar to nitrogen, phosphorus transport in a catchment involves runoff, erosion and leaching. However, due to its highly adsorptive characteristics, phosphorus leaching is not the main focus in most of the studies. Especially when strong rainfall event occurs, and few events can contribute over 90% of annual phosphorus loads (Sharpley (1995). There is also the concern that the overland flow during catastrophic events generate soil loss accompanied by particulate phosphorus (Leinweber et al., 2002). Transport of dissolved and particulate phosphorus is modelled in a similar manner as nitrogen compositions presented in the previous section 2.3.5.2 “Nitrogen loss.”

2.5. River water quality routing

In the previous section of this chapter, the main processes relating to nutrient generation, transformation and transport in upland areas were given. The nutrients arrive into the channel network, where they are deposited, and transported down stream. Other sources like bank eroded materials or wastewater discharge are also added to the network. While hydrology-related factors are dominant in the upland areas, hydraulic factors govern in the down streams, and the transition areas involve both hydrological and hydraulic aspects (Chow et al., 1988). In this section, water flow routing is first introduced. It serves as driving means for nutrient transport. Second, a description of sediment routing through river network is given. Third, nutrients in both particulate and dissolved forms routed along

the river networks are presented. Finally, the section ends with “Collection of river water quality data” where measurement techniques as well as associated errors are discussed.

2.5.1. River routing

Flow routing is used to determine the time and magnitude of flow at a point in the river network given inflow from upstream areas (Chow et al., 1988). Depending on the complexity of the system, the flow can be routed as lumped or distributed. In lumped routing, flow is calculated as a function of time at a particular location (e.g. catchment outlet), while in distributed routing, flow is calculated as a function of time and space depending on discretization schemes

2.5.1.1. Distributed flow routing (hydraulic routing)

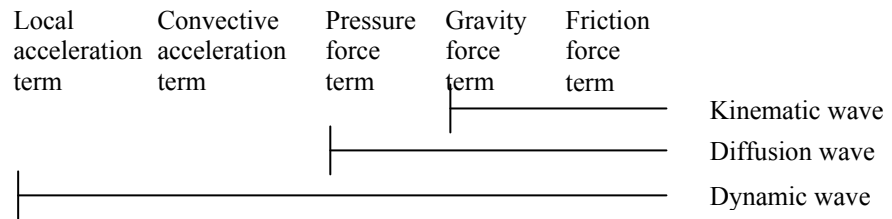
The distributed flow routing or hydraulic routing basically combines the continuity equation with the physical movement of the water expressed as the momentum equation. In distributed flow routing analysis, the dynamics of the water or flood wave movement can be rather accurately described. Chow et al. (1988) presents the these two equations as the Saint-Venant equations for one-dimensional, unsteady flow as follows:

Continuity equation (Conservation form):

$$\frac{\partial Q}{\partial x} + \frac{\partial A}{\partial t} = 0 \quad (\text{eq. 2.46})$$

Momentum equation (Conservation form):

$$\frac{1}{A} \frac{\partial Q}{\partial t} + \frac{1}{A} \frac{\partial}{\partial x} \left(\frac{Q^2}{A} \right) + g \frac{\partial y}{\partial x} - g(S_0 - S_f) = 0 \quad (\text{eq. 2.47})$$



Detail descriptions for each term are presented in terms of the kinematic, diffusion and dynamic wave equations.

Dynamic wave equations

The basic flow-governing equations are the dynamic wave equations, often referred to as the St. Venant equations or shallow water wave equations. These consist of the equations of continuity and momentum for gradually varied unsteady flow respectively expressed as:

$$\begin{aligned} \frac{\partial Q}{\partial x} + \frac{\partial h}{\partial t} &= 0 \\ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + g \frac{\partial h}{\partial x} &= g(S_0 - S_f) \end{aligned} \quad (\text{eq. 2.48})$$

Where:

- A = Average cross-sectional area (m²)
h = Flow depth (m)

Q	=	Flow per unit width (m ³ /s/m)
u	=	Water velocity (m/s)
g	=	Acceleration due to gravity (m/s ²)
S ₀	=	Bed slope (m/m)
S _f	=	Energy gradient (m/m)
t	=	Time (s)
x	=	Longitudinal distance (m)

There is no analytical solution of these equations. Approximate numerical solutions of these two equations have been implemented in river flood routing models such as the implicit finite difference scheme (e.g. see in Chapra and Canale, 2002).

The dynamic wave equations have not been used in catchment models because of their computationally intensive numerical solutions.

Diffusive wave equations

Diffusive wave equations consist of the equations of continuity and momentum, expressed as

$$\begin{aligned}\frac{\partial Q}{\partial x} + \frac{\partial h}{\partial t} &= q \\ \frac{\partial h}{\partial x} &= g(S_0 - S_f)\end{aligned}\quad (\text{eq. 2.49})$$

Where:

$$q = \text{lateral inflow per unit width and per unit length (m}^3\text{/s/m/m)}$$

This continuity equation includes lateral inflow. The simplified momentum equation expresses the pressure gradient as the difference between the bed slope and the energy gradient, and is derived from the Saint-Venant equation after ignoring the first two terms, representing respectively the local and convective acceleration.

Similar to the dynamic wave equations, there is no analytical solution for the diffusive wave equations. In solving these equations, Manning's formula is used to compute flow, which is expressed as:

$$Q = \frac{1}{n} A R^{2/3} S_f^{1/2} \quad (\text{eq. 2.50})$$

Where:

n	=	Manning's roughness coefficient
A	=	Flow cross-sectional area per unit width (m ² /m)
R	=	Hydraulic radius (m)

Kinematic wave equations

The kinematic wave equations are the simplest form of the dynamic wave equations. Kinematic wave theory is now a well-accepted tool for modeling a variety of hydrological process (Singh, 1996). Kinematic wave equations consist of the continuity equations and the simplest form of the momentum equation after ignoring all the acceleration and pressure gradient terms in the Saint-Venant equations, respectively expressed as equations 2.7, and 2.8:

$$\frac{\partial Q}{\partial x} + \frac{\partial h}{\partial t} = q$$

$$S_0 = S_f$$

The second momentum equation is expressed simply as the energy gradient equal to the bed slope. Any suitable law of flow resistance can be used to express this equation as a parametric function of the stream hydraulic parameters. A widely used expression is:

$$Q = \alpha h^m \quad (\text{eq. 2.51})$$

Where α is the kinematic wave parameter, m is the kinematic wave exponent, α and m are roughness and geometry, respectively.

The advantage of these equations is that they have an analytical solution, which can be found by using the method of characteristics (Borah et al., 1980).

2.5.1.2. Lumped flow routing (hydrologic routing)

For a hydrologic routing system, input $I(t)$, output $Q(t)$, and storage $S(t)$ are described by the continuity equation

$$\frac{\partial S}{\partial t} = I(t) - Q(t) \quad (\text{eq. 2.52})$$

If the inflow hydrograph $I(t)$ is known, this equation can not be solved directly to obtain the outflow hydrograph $Q(t)$ because both Q and S are unknown. A second relationship or storage function relating S , I and Q is needed. Coupling the storage function with the continuity equation provides a solvable set of two equations and two unknowns. Chow et al. (1988) lists a number of available routine techniques such as:

- Level pool routing
- Muskingum method
- Linear reservoir model

2.5.2. Sediment river routing

Certain nutrient contaminants can be transported through the river network with the sediment, e.g. Phosphate, or organic matters since they can be adsorbed or desorbed into the sediment. Thus, knowledge about sediment routing in river network cannot be neglected in the study nutrient transport.

Sediment routing in river network is complicated especially due to the interaction between river flow and channel morphology, i.e. channel bed and channel bank. Thus, transported materials include eroded sediments not only from upland catchment but also from the river itself. Based on the mechanism of sediment transport, it is possible to classify the transported sediment into suspended and bed loads. Bedload sediment moves along the bottom of the flow and can be limited in deposition, while suspended load is distributed throughout the flow (Foster, 1982). However, according to sediment sizes, the wash load in the top of the surface water as can be seen in Figure 2.17. The washload i.e. (dominant) clay, is mostly contributed by the upland erosion (Foster, 1982; Obermann, 2007). Thus, sediment yield collected at outlet in the top of the surface water can be assumed to be the result of upland erosion.

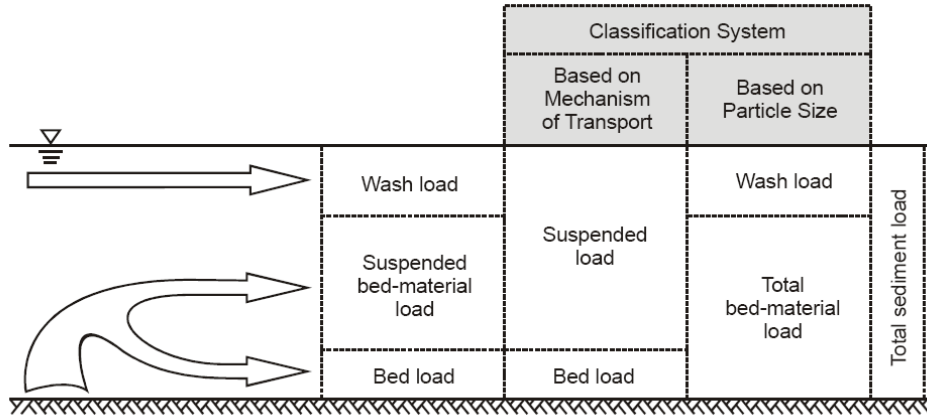


Figure 2.17: Classification of sediment transport (Obermann, 2007)

Similar to the description of sediment transport on land surface in section 2.2.2.8 “sediment routing on overland,” the transport of sediment in river primarily depends on (1) actual transport capacity (mainly as a function of flow parameters), and (2) the critical transport capacity (mainly dependent on sediment properties) (Obermann, 2007).

Detailed processes of sediment transport in a river network is rather complex due to many aspects involved, e.g. hydrodynamic, river morphology, and is out of the scope of this thesis. Standard textbooks dealing with sediment transport mechanisms can be found in various in literature (e.g. in Graf, 1971; Julien, 1995; Yang, 1996). A few selected model algorithms for transporting wash load or suspended load that have mostly been implemented in catchment water quality models are shown below.

The Bagnold stream power concept (in Yang, 1996), suspended load can be computed as

$$\frac{\gamma_s - \gamma}{\gamma} q_{sw} = \frac{0.01 \tau V^2}{\omega} \quad (\text{eq. 2.53})$$

Where:

- γ_s = Specific weights of sediments
- γ = Specific weights of water
- q_{sw} = Suspended load discharge in the dry weight per unit time and width
- τ = Shear force acting along the bed
- V = Average flow velocity
- ω = Fall velocity of suspended sediment

Sediment mass conservation (Bennett, 1974; modified in Lukey et al., 1995)

$$\frac{\partial(Ac_i)}{\partial t} + (1 - \phi)B \frac{\partial z_i}{\partial t} + \frac{\partial G_i}{\partial x} = q_{si} \quad (\text{eq. 2.54})$$

Where:

- A = Flow cross sectional area (m^2)
- C_i = Concentration of sediment particles in size group i (m^3/m^3)

- ϕ = Bed sediment porosity
 B = Active bed width for which the is sediment transport(m)
 z_i = Depth of bed sediment (m)
 G_i = Volumetric sediment transport rate for the sediment size fraction (m^3/s)
 q_{si} = Represent sediment input from bank erosion and overland flow supply per unit channel length for size fraction i ($m^3/s/m$)

This sediment continuity equation is coupled with the Saint-Venant equations as already previously presented.

2.5.3. Contaminant river routing

The nutrient routing in river mainly involves two groups: transport and transformation. Two primary transport modes are **advection** (transport associated with the flow of a fluid) and **diffusion** (transport associated with random motions within a fluid). Transformations are processes that change a substance into another. Transformations can be driven by either physical processes (e.g. radioactive decay) or chemical or biological reactions such as dissolution. In addition, the sources of nutrients that reach the river network as well as nutrient losses during transportation are taken into account in nutrient routing (Chapra, 1997; Lin and Falconer, 2005; Socolofsky and Jirka, 2002).

A governance equation in one dimension used to describe the contaminant (C) routing is the advection-diffusion equation as follow:

$$\frac{\partial C}{\partial t} + \frac{\partial u_i C}{\partial x_i} = D \frac{\partial^2 C}{\partial x_i^2} \pm R \quad (\text{eq. 2.55})$$

In the left equation, the first term is temporal changes; second term is advection transport. In the right equation, the first term is diffusion transport and the second-grouped term account for all transformation processes and sources or sinks.

Since equation 2.55 is a fully-formed equation applied in modeling contaminant transport in a river. However, it may not be necessary to use the equation for cases since some processes may be dominant to others as shown in the following.

2.5.3.1. Advection/dispersion components

$$\frac{\partial C}{\partial t} + u_i \frac{\partial C}{\partial x_i} = D \frac{\partial^2 C}{\partial x_i^2} \text{ is the form of the advection diffusion equation.}$$

Diffusion versus advection dominance is a function of t, D and u, and this property is presented as the non-dimensional Peclec number.

$$Pe = \frac{D}{u^2 t} \text{ or for a given downstream location } L=ut,$$

$$Pe = \frac{D}{uL} \quad (\text{eq. 2.59})$$

Where:

- D = Diffusion coefficient
 u = Flow velocity
 L = Length scale

For $Pe \gg 1$, diffusion is dominant and the contaminant spreads out faster than if it moves downstream; for $Pe \ll 1$, advection is dominant the cloud moves downstream faster than it spreads out: for large times or distances, the Peclet number is small and advection dominates (Socolofsky and Jirka, 2002).

2.5.3.2. Advection dominance: Plug-flow reactors

For $Pe \rightarrow 0$ we can neglect longitudinal diffusion and dispersion, and we have plug flow reactor. Thus, $D=0$, the governing reactive transport equation becomes:

$$\frac{\partial C}{\partial t} + u_i \frac{\partial C}{\partial x_i} = \pm R \quad (\text{eq. 2.60})$$

2.5.3.3. Diffusion dominance: Continuously-stirred tank reactors (CSTR)

For $Pe \rightarrow \infty$ advection can be neglected leading to the continuous-stirred tank reactor (CSTR). Fluid enters the reactor and is assumed to instantaneously mix throughout the reactor.

$$\frac{dM}{dt} = m_{in} - m_{out} \dots \rightarrow \frac{dC}{dt} = \frac{1}{t_{res}} (C_{in} - C) \pm R \quad (\text{eq. 2.61})$$

2.5.3.4. Tank-in-series model

A river can be modelled by incorporating the diffusion or dispersion in the tanks-in-series model. This will form a chain of linked CSTRs. An example tanks-in-series model is shown in Figure 2.18. In the example each tank has the same dimensions and the flow rate is constant.

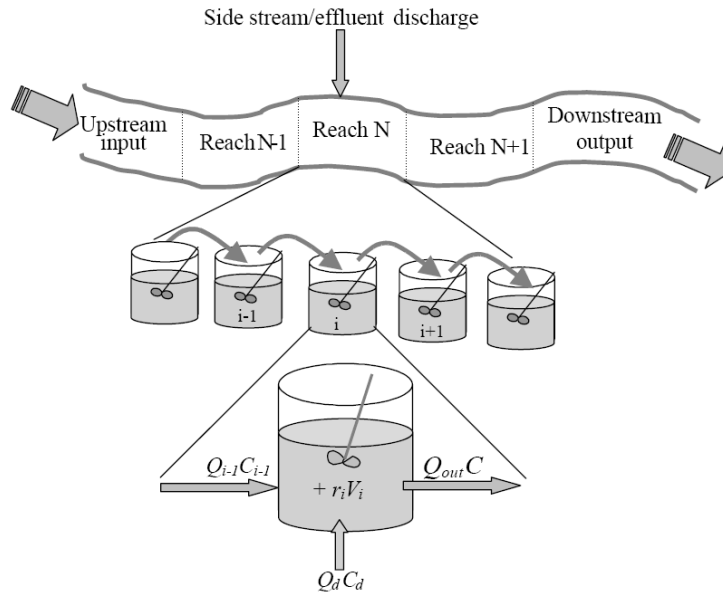


Figure 2.18: River discretization, a cascade of CSTRS model and mass balance (Tolessa, 2004)

The method also works for variable volume tanks and under gradually-varied flow conditions, stage-discharge relationship can be used to route variable flows through the tanks.

$$\frac{dM_i}{dt} = Q(C_{i-1} - C_i) \pm VR \quad (*) \quad (\text{eq. 2.62})$$

If the reaction term R is neglected based on a number of processing steps as described in Socolofsky and Jirka (2002), the formula (*) becomes:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = \frac{u \Delta x}{2} \frac{\partial^2 C}{\partial x^2} \quad (\text{eq. 2.63})$$

This is the advection diffusion equation, with the diffusion coefficient $D = \frac{u \Delta x}{2}$.

The effective diffusion coefficient, D , for a tanks-in-series model is actually is a numerical error due to the discretization. As discretization become coarser, the numerical error increases and the numerical diffusion go up. For $\Delta x \rightarrow 0$, the numerical diffusion vanishes, and we have the plug-flow reactor. Hence, for a tank-in-series model, we choose the tank size such that D is equal to the physical longitudinal diffusion and dispersion in the river reach.

Further discussions about plug flow and CSTR model such as the comparison between plug flow and CSTR model can be found in Wilson et al.(1986), or Bendoricchio and Rinaldo (1986), Bicknell et al. (2001) for the implementation of the CSTR model in catchment modeling.

2.5.3.5. Reaction kinetics

Substances in water experience different processes including physical, chemical, and biological in different fates. Understanding this conversion is essential in water quality model. This transformation is popularly expressed with reaction kinetics which can usually be classified into zero-order, first order and second order reactions.

Zero-order reactions

Zero-order reactions are independent of the concentrations of the reacting elements. The reaction rate is constant:

$$\frac{dC}{dt} = \pm k, \quad (\text{eq. 2.64})$$

Where:

- c = Concentration [ML^{-3}]
- t = Time [T]
- k = Zero order rate constant [$\text{ML}^{-3}\text{T}^{-1}$]

Thus concentration variation will not change the rate of the reaction. An example of this reaction is a photochemical reaction.

First-order reactions

The general equation for a first-order reaction is

$$\frac{dC}{dt} = \pm kC \quad (\text{eq. 2.65})$$

Where:

- k = Constant [T^{-1}], e.g. radioactive decay and the dye-off of bacteria in a river.

Applying the initial condition, C_0

$$C(t) = C_0 \exp(\pm kt)$$

Second-order reactions

The general equation for a second-order reaction is

$$\frac{dC}{dt} = \pm kC^2 \quad (\text{eq. 2.66})$$

Where:

$$k = \text{Constant } [L^3 M^{-1} T^{-1}].$$

This is another initial-value problem, which can be solved given the initial condition

$$C(t=0) = C_0$$

Solving $C(t)$ gives:

$$C(t) = \frac{1}{\mp kt + 1/C_0}$$

Higher-order reactions

The general equation for an n^{th} -order reaction is

$$\frac{dC}{dt} = \pm kC^n \quad (\text{eq. 2.67})$$

Where:

$$k = \text{Constant } [L^{3(n-1)} M^{-(n-1)} T^{-1}].$$

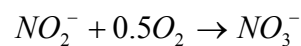
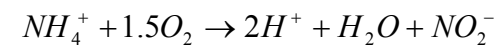
The general solution given the initial condition $C(t=0) = C_0$ is

$$\left(\frac{1}{(n-1)} \right) \left[\frac{1}{C^{n-1}} - \frac{1}{C_0^{n-1}} \right] = kt$$

The higher order reactions are rare, and different values of n can be used in a reiterative process to find an equation that best fits the experimental data.

Examples of kinetic reactions of nutrient in water

Chapra (1997) presents nitrification modeling, where assuming first-order kinetics, the nitrification process can be written as a series of first-order reactions.



$$\frac{dN_a}{dt} = -k_{oa}N_o - K_{ai}N_a$$

$$\frac{dN_i}{dt} = -k_{ai}N_a - K_{in}N_i$$

$$\frac{dN_n}{dt} = -k_{in}N_i$$

The subscripts o, a, i, and n denote organic, ammonium, nitrite, and nitrate, respectively.

2.5.4. Collection of river water quality data

River water quality data is substantial, for example, to assess the water quality or to be used for calibration and validation of simulation results. However, available observations from responsible agencies are often limited in temporal scale (e.g. maximum daily time steps, discontinuity) as well as spatial distribution. Finer resolution is often done at field scale (few hectares) or small catchment ($< 5 \text{ km}^2$) for research purposes (e.g. in Cooper et al., 2007; Inamdar et al., 2006; Salles et al., 2008). Flood event are so a big challenge for data collection. Extremely harsh working environment and damages caused by flood (e.g. discussed in Manley and Askew, 1993) are the main reasons that limit data available to assess impact of storms. Furthermore, treatment to nutrient variation during flood event is often based on statistical analysis (e.g. House and Warwick, 1998; Stutter et al., 2008) which is not easy to perform when dealing with complex system, especially under various anthropogenetic impacts (Højberg et al., 2007). Therefore, a proper collection of water quality data is essential in catchment water quality modeling.

Collection of water quality data presented follows the description presented by Harmel et al. (2006a). An example of a sampling strategy for the determination of nitrogen concentration is illustrated in Figure 2.19. The collection includes four procedural categories: streamflow (discharge) measurement, sample collection, sample preservation/storage, and laboratory analysis.

Discharge measurement

Discharge measurement is important in water monitoring program. Discharge data is used not only to assess stream flow conditions (e.g. drought or flood) that are vital for water balance perspective, but also to combine with constituent concentration data to calculate loadings that is a base for waste water allocation purpose. Flow discharge data is obtained by combining river cross section and flow velocity (Herschy, 1995) with the help of a stage – discharge relationship. Cross section can be drawn during low flow condition. Flow velocity can be measured using a current meter at different flow depths or by using the advanced Acoustic Doppler Current Profiler (ADCP). Based on a number of observed discharges and water levels, a stage – discharge curve can be developed. After a obtaining a certain confidence, e.g. 95%, flow velocity is no longer needed, and only water levels are recorded. Currently, an automatic streamflow measurement station operates based on recording water levels. However, due to changes of stream morphology e.g. bank erosion bed scour or deposition, the relation of stage and discharge should be re-estimated after a few years. In many cases – in particular in tropical regions, the error of flood flow data is extremely high (Meon and Hildebrand, 2010)

Sample collection

Water sampling can be done either with manual sampling or automatic sampling. Issues of concern in sampling activities are sampling frequency and sample composites. In manual sampling, sampling composite can be done by the Equal-Width Increment method (EWI) and Equal-Discharge Increment (EDI) method (Harmel et al., 2006a). These methods take multiple depth-integrated, flow-proportional samples across the stream cross-section and produce accurate measurements of dissolved and particulate concentrations (Harmel et al., 2006a). The higher frequency of manual sampling, the higher the effort is required. By automatic sampling, the frequency is not problematic since it can be set up from sampling equipment. However, automatic sampling is usually implemented with a single intake only. Harmel et al. (2006b) introduce potential advantages and disadvantages of automated and manual storm sampling as shown in Table 2.7

Sample preservation/storage

Water quality data can be affected by preservation or storage techniques. Physical, chemical, and biological processes can alter nutrient concentrations (Harmel et al., 2006a). Pre-treatment of water sample as well as the storing facility (e.g. plastic/glass bottle, refrigeration) are required (e.g. described in Bartram and Ballance, 1996). For analyzing dissolved contaminants, filtering sample immediately or shortly after sampling is also very important. To distinguish between dissolved and adsorbed nutrient, a 0.45µm filter is commonly used, see (Sharpley, 2007).

Laboratory analysis

Laboratory analysis for nutrient concentration often follows the methods described in “Standard methods for the examination of water and wastewater” (2005), e.g. see Figure 2.20. In addition, in situ methods using photometer (e.g. from Spectroquant NOVA 60) are also practical in remote areas.

Table 2.7: Potential advantages and disadvantages of automated and manual storm sampling (Harmel et al., 2006b)

Automated Storm Sampling		Manual (EWI or EDI) Storm Sampling	
Advantages	Disadvantages	Advantages	Disadvantages
Reduced on-call travel.	Large investment in equipment.	Low equipment cost.	Frequent on-call travel often needed in adverse weather conditions.
Multiple samples collected automatically.	Single sample intake (samples taken at one point in the flow).	Integrated samples throughout.	Time-consuming travel and sample collection make multiple sites difficult to manage.
Minimizes work in dangerous conditions.	Difficult to secure intake in centroid of flow.	Vertical profile and cross-section.	Difficult to obtain samples throughout hydrograph.
Numerous sites feasible.			Large investment in personnel.

It should be noted that Harmel et al. (2006a) conducted a review on uncertainty of water quality data. They found that the probability of error of these data can range from a few to more than 100 percent. Therefore, a sound judgement on the available data is critical before using them for model calibration and validation, or statistical analysis. An approach based on the root mean square error propagation method can be used (Topping 1972, cited in Harmel et al., 2006a). Cumulative errors of measured data can be calculated as:

$$E_p = \sqrt{\sum_{i=1}^n (E_1^2 + E_2^2 + E_3^2 + \dots + E_n^2)} \quad (\text{eq. 2.68})$$

Where:

- E_p = Probable range in error ($\pm\%$)
- n = Total number of sources of potential error
- $E_1, E_2, E_3, \dots, E_n$ = Probable range in error ($\pm\%$) for sources 1, 2, ..., n

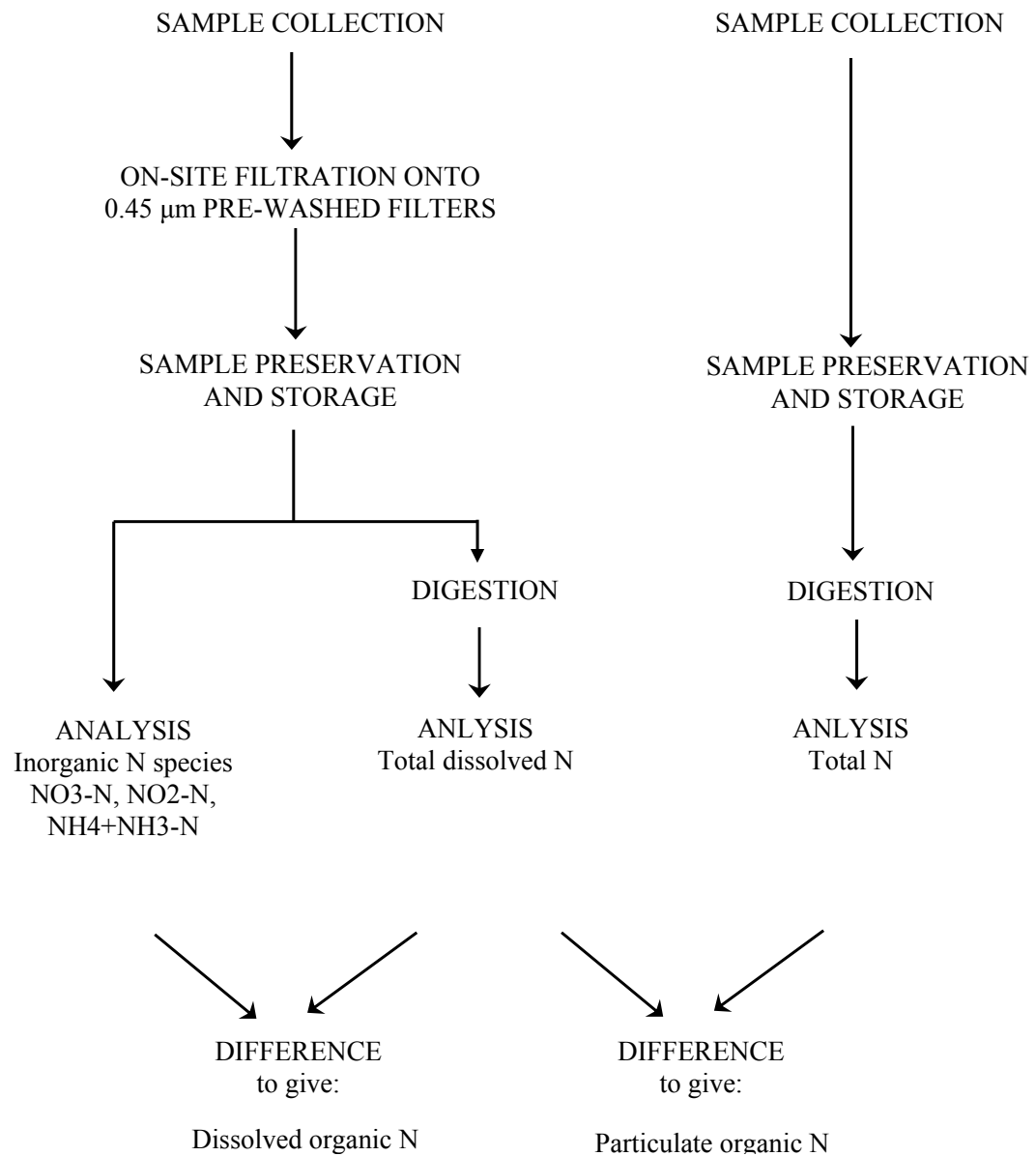


Figure 2.19: General sampling strategy for determination of nitrogen concentration (Johnes and Burt, 1993)

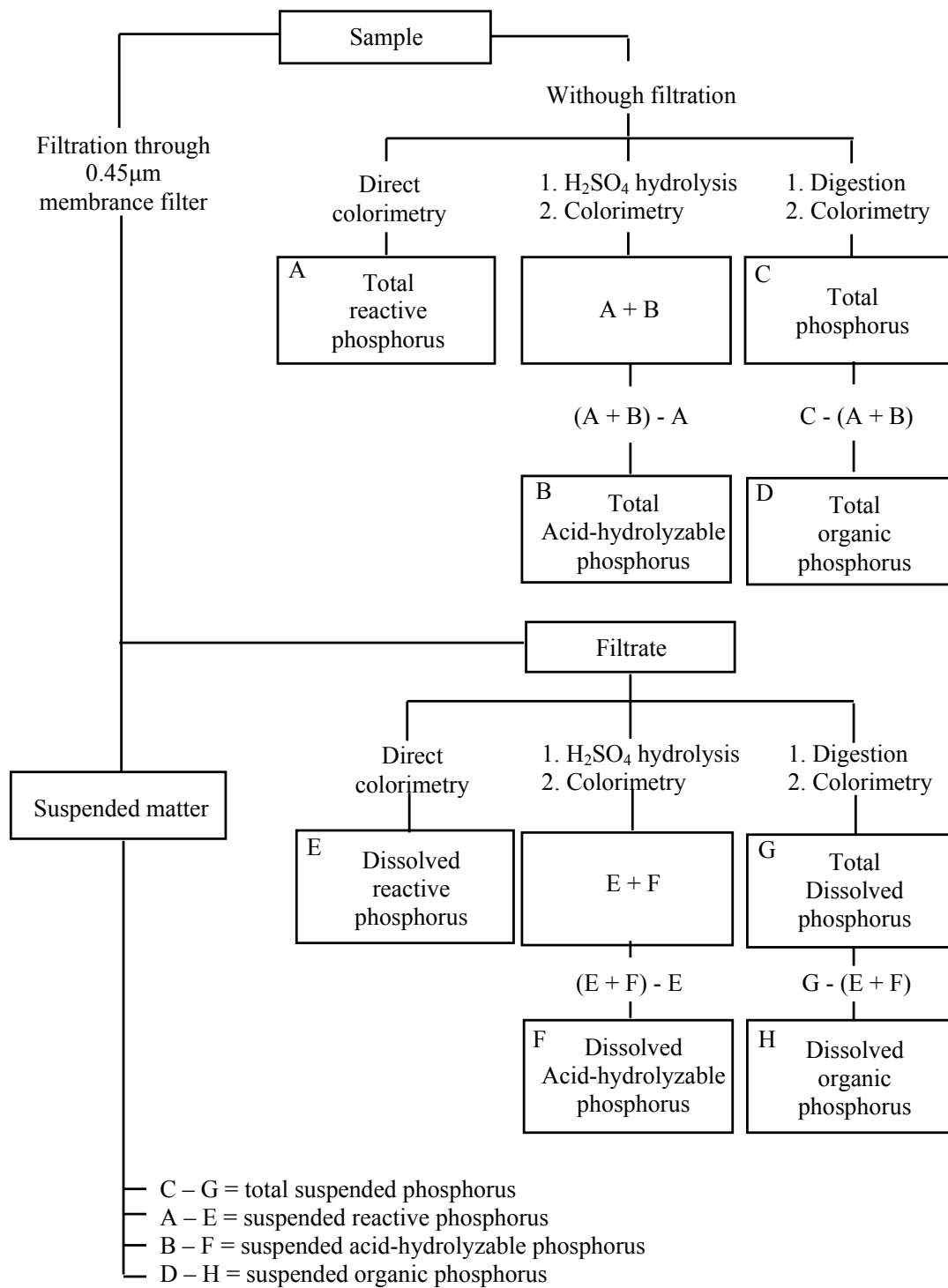


Figure 2.20: Steps for analysis of phosphate fraction (Standard methods for the examination of water and wastewater, 2005)

2.6. Approaches to catchment water quality modeling

In the previous sections of this chapter, catchment processes as well as model algorithms are provided. However, to link these processes with the help of a model covering all the components, requires an understanding of more issues. The following section is devoted to these additional issues.

In this section, first, an overview on different types of models is presented. This is followed by an identification of the current modeling issues. The “uncertainty analysis” in modeling is provided next. Finally, a selection of available model codes is presented.

2.6.1. Model classification ⁶

Since the development of computer science, modeling approaches involving computer programs have rapidly increased in different fields, and this is also true for catchment modeling. A model according to system theory and its properties can be seen in Figure 2.21. The abstracted model of reality is limited by a model boundary, an interface between modeling system and the surrounding environment. In order to describe a system, a model usually contains constant coefficients, parameters as well as state variables. The variation of the system is caused by the change of input variables. Consequently, certain information can be obtained as output variables.

Catchment modeling involves diverse processes leading to numerous model parameters and variables which are presented in different mathematical forms. Due to the complexity and high variation of the system, catchment modeling approaches are basically classified into two main categories. The first one is a stochastic model where model inputs, parameters or variables do not have fixed values at a particular point in space and time. In other words, they are probabilistic or random. The second type is the deterministic model which does not or only indirectly take into account the randomness. For given model input data, model parameters always produce the same output (Chow et al., 1988).

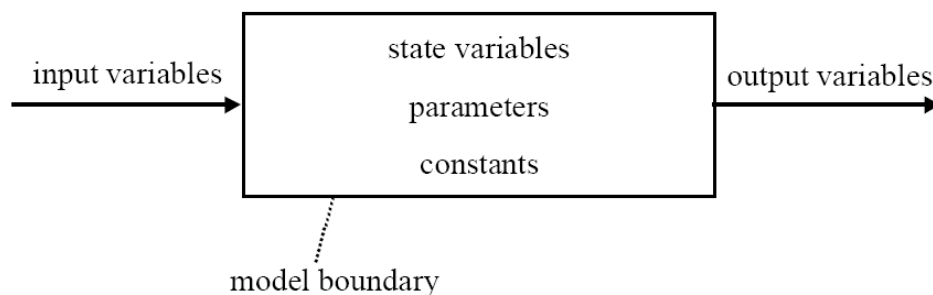


Figure 2.21: Model and model properties according to system’s theory (Bierkens, 2006)

2.6.1.1. Stochastic models

Novotny and Olem (1994) state that stochastic does not mean “completely random.” A stochastic modeling system can contain both deterministic and stochastic aspects (Box and Jenkins, 1976, cited in Novotny and Olem, 1994). In catchment water quality modeling, the stochastic model is often seen in simulation of separated processes such as transformation of excess rainfall to runoff (e.g. in HBV model, Bergstrom, 1995) or contaminant leaching in soil (Addiscott and Wagenet, 1985; Jury and

⁶ It is restricted in computer model only; another model type that is physical model (Chow et. al., 1988) is not considered.

Horton, 2004, chapter 7) using transfer functions. Novotny and Olem (1994) classify stochastic models by 2 types: (1) univariate ARMA; and (2) transfer function (including both single input – single output and multiple input – single output). An example of a stochastic model is shown in Figure 2.22. In this thesis, not much attention is given to stochastic models.

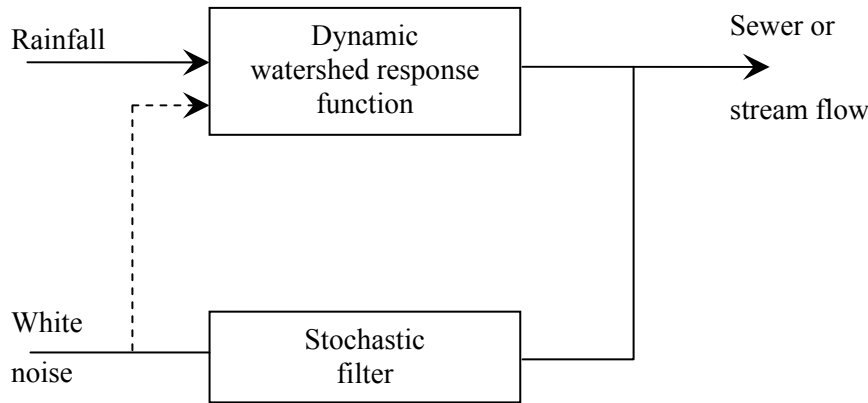


Figure 2.22: Representation of stochastic modeling system. In addition to rainfall, other input may also be considered (Novotny and Olem, 1994)

2.6.1.2. Deterministic models

Basically, when considering deterministic models and its complexity, the following main types are available:

- Empirical model
- Physically-based model
- Conceptual model

In the following sections, these three models are only briefly described. Comprehensive review on these subjects can be found in the literature (e.g. in Aksoy and Kavvasb, 2005; Chow et al., 1988; Dooge, 1977; Merrit et al., 2003; Rientjes, 2004; Singh, 1995a; Zhang et al., 1996).

Empirical (black box) models are based primarily on the analysis of observations. Later, equations are set up to relate these observed data. The models contain parameters that may have physical characteristics that allow the modeling of input-output patterns based on empiricism. However, empirical models do not aid in physical understanding. The dominant character of these models is their simple representation of the system in both time and space. They require limited model data (input and parameters). Empirical models are preferred in limited data areas. Examples of this approach are the unit hydrograph, rational method, etc. which are applied to the whole catchment as a lumped system (black box) and are well described in Singh (1988), Merrit et al. (2003)

Physically based (or theoretical, white box) models are based on fundamental physical laws that include a set of conservation equations of mass, of momentum, of energy and specific case of entropy to describe the real world physics, e.g. streamflow, sediment and associated nutrient generation. The first two equations are most popularly applied in current models. Examples of this approach are SHE (Abbott et al., 1986), and REW (Reggiani and Rientjes, 2005). Since the physically-based models

attempt to present the system in great details, the models are highly parameterized and various data are required for running the model, These data are often not available.

Conceptually based (grey box) models consider physical laws but in a simplified form, i.e. the conservation of mass. The conceptual model represents a catchment system typically as a series of internal storages, through which the general processes of the system are conceptualized without describing specific details of interactions (Merrit et al., 2003). The conceptual models can function as a transition model between empirical and physical-based models. Although the conceptual model looks at the system as consisting of separated components, it much reflects the underlying processes of the system behaviour. This feature makes the conceptual models more advanced than empirical models. Examples of this approach are found in some model such as Tank (Sugawara, 1995), Sacramento (Burnash, 1995), TOPMODEL (Beven et al., 1995), HBV (Bergstrom, 1995), NAXOS (Riedel, 2004).

2.6.1.3. Other model classification scheme

Model types according to spatial distribution

The catchment system is not homogeneous. Its characteristics are distinguished because of spatial variation not only on the surface, i.e. land cover, landuse, and geomorphology but also underground, i.e. soil profiles. Considering these spatial variations in terms of processes and parameters, models can be classified as the following groups:

- Lumped models
- Distributed models
- Semi-distributed models

This classification scheme is very popular because it is not difficult to partition the system with modern techniques like Geographic Information System (GIS), or spatially distributed data through Remote Sensing (RS). Additional information of these types of models can be found in (Cunderlik, 2003; Merrit et al., 2003), hereunder they are briefly described as follows:

Lumped models

In the lumped models, parameters do not vary spatially within the catchment. The system response is evaluated only at the catchment outlet. Interactions between sub-catchments are not explicitly considered. Parameters of lumped models are often not directly measured from the field, a truly physical representation is missing. They are usually obtained by empirical approach and aggregated over the whole catchment in order to get affective values. The lumped models are popularly found in empirical models and conceptual models as discussed in the previous sections. The models are very useful and commonly applied when detailed data is not available or when requirements to the modeller are not high, e.g. discharge in the outlet only. Typical limitation of the models is, of course, the limited physical representation of the system leading to extreme difficulty in management activities, e.g. land use planning for Best Management Practice.

Distributed models

In the distributed models, model parameters vary spatially in the catchment. The uniform parameter is only at the model resolution which is in grid based models, e.g. a grid cell size defined by modellers. Distributed modeling approach can include/model all the details in the system, thus data is extensively required, although they are not often available. Physically-based models best complement the

distributed models since they represent the “real” physical characteristics of the system. If data is available, and these models are properly used; these models are expected to produce the most accurate model behaviours. Therefore, distributed models are basically best suited to management purposes e.g. Best Management Practice. Examples of distributed models are physically-based models such as SHE (Abbott et al., 1986), KINEROS (Woolhiser et al., 1990), WEPP (Flanagan and Nearing, 1995) or the simple distributed ANGPS model (Young et al., 1989). However, lack of input data and enormous computation times often limit application of physically – based models in the praxis.

Semi-distributed models

Semi-distributed models are located somewhere in between the lumped and distributed models. In semi-distributed model, parameters vary spatially in the catchment with the smallest unit as sub-basin or land use. Regarding data issues, semi-distributed models can compromise the lumped and distributed models since data for semi-distributed models are mostly available. The lumped models often accompany the conceptual model as seen in HSPF (Bicknell et al., 2001), or SWAT (Arnold et al., 1994), although they can be implemented in physically-based model, e.g. REW (Reggiani and Rientjes, 2005; Reggiani and Schellekens, 2005).

Model types according to temporal discretization

Regarding temporal changes of model inputs and outputs, or how the system responses according to time, models can be classified into: (1) Steady state, (2) Quasi-dynamic, (3) Dynamic (Chow et al., 1988; Shoemaker et al., 2005). In steady state, variables do not vary according time, i.e. there is no time derivative in the model equations. With respect to the quasi-dynamic model, variables change with time in a limited variation, i.e. coarse time steps. Finally, in dynamic or unsteady models, there is no limitation in temporal variations in model implementation. There are some illustrations of this type of model classification in the book written by Chow et al (1988).

Event-driven models and continuous-process models are also classified according to the time scale. However, these are limited to total period of simulation. The event models look at the change during a short time period, e.g. few hours during flood events, whereas the continuous models capture how the systems changes in longer periods, for example, years.

2.6.2. Integrated catchment water quality model

As presented in sections 2.2.1 - 2.2.5 of this chapter, catchment water quality modeling involves various processes crossing different spatial and temporal domains. Arheimer and Olsson (2003) lists several model categories, including catchment scale model; river channel model; soil water and field scale model, as ones that are most closely related to catchment water quality modeling. Depending on research objectives, and especially system complexity, model domains should be linked and coupled at a certain level, for example, as recommended in the HarmonIT project (Hutchings et al., 2002) where linked model domains are proposed including (1) Soil processes; (2) Run-off; (3) Groundwater flow; (4) Surface Water flow; (5) Water chemistry; (6) Ecological processes; (7) Economic considerations. A reference is made to the work of Newham et al. (2004) where four components are integrated into one framework, i.e. hydrologic, economic, sediment and nutrient export models. The coupled modeling framework will be at the core of integrating catchment modeling system and will also be helpful for the integrated catchment management. Figure 2.23 illustrates how model domains relate with different modeling groups. In addition, as recommended by (Refsgaard et al., 1998) and

Lindenschmidt et al.(2007), an integrated modeling system will reduce model uncertainty due to, for example, closing internal boundary of model domains, explicitly presenting sources of data

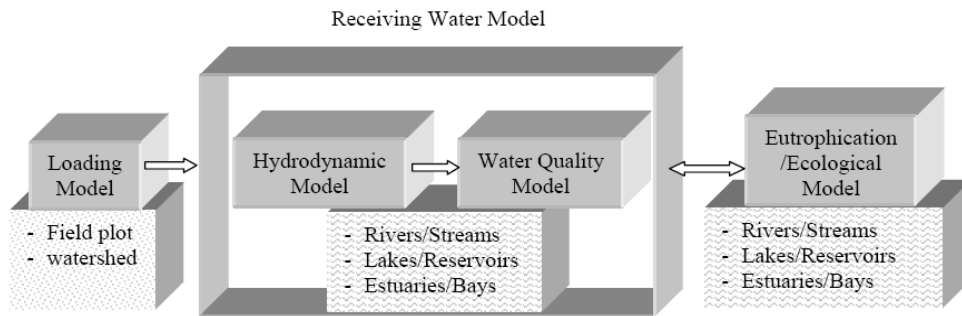


Figure 2.23: Relationship between different model groups (Kalin and Hantush, 2003)

2.6.2.1. Levels of model coupling systems

Lindenschmidt (2005) looks at the levels of couple model including ease, applications, etc. and classifies the coupled models into the following three types, while Imhoff et al. (2003) only uses two types (loose and tight coupling).

Loosing coupling system is the conventional type of coupled models where the links between model domains are loosely coupled. The system operates as follows: results of one model are stored in files and transferred to another model. Implementation of this coupled type does not require programming in model source codes. Sequence control is managed by batch files or an external program. This coupling type is found in many applications such as surface water and groundwater interaction eg. in (Kim et al., 2008) or (Koch et al., 2007); catchment and water body models (Debele et al., 2008; Wu et al., 2006).

A coupling platform, which can be considered as a transition between loose and tight coupling system, is a system in which model domains are integrated into the simulation environment. Because several steps in system execution are similar, and would be repeated, the efficiency of model simulation may be reduced. Interacting with the model source code is required in order to improve simulation speed. An example of this coupling style is HLA (High Level Architecture) (Lindenschmidt, 2005; Lindenschmidt et al., 2005).

An object oriented modeling system is the most advanced coupling system in which sub-models are separated as single processes (tight coupling system). A sub-models runs only when it is called for a certain modeling step. It is required to know model source codes so that each sub-model can be implemented as an object. Thus, developing such a system is extensively hard although its efficiency is high. Several water modeling system have been developed for use like MOHID (ready-to use) (Braunschweig et al., 2004), OPENMI as a framework for integrating other models) (Gregersen et al., 2007).

Although advantages of model coupling are abundant, a number of issues still exist in developing a coupling system (Gijssbers et al., 2002; Imhoff et al., 2003). For example:

- Spatial and temporal scale matching
- Processes formulation incompatibility

- Dependent on model domains (e.g. Difficulties in coupling catchment loading with tidal-affected river model)
- Operational problems (data exchange mechanisms, run time between models)
- Lacking of common data definition in different model domains

2.6.2.2. Integrated catchment water quality model, an example of the BASIN modeling system

A movement towards a practical tool that assists a water resources manager is the ultimate aim of all water modeling systems. Shoemaker et al. (2005) define an integrated system in water resources management to include a (1) data support system; (2) multiple model choices; (3) data analysis tools; (4) consistency and efficiency in linking of data to model as well as from one model to another. Better Assessment Science Integrating point and Nonpoint Sources (BASINS) (US EPA, 2007) is a typical illustration. Promotion of this modeling system can be found in large number in the literature, e.g. “BASINS was considered to be an excellent beginning tool to meet the complex environmental modeling needs of the 21st Century” (Whittemore and Beebe, 2000) or in “*BASINS 4.0* - Flexible Integration of Components and Data for Catchment Assessment and TMDL Development” (Duda et al., 2003.)

The system (see Figure 2.24) includes the following advances that lead to its increasing usage in water modeling practices:

- Open source GIS software architecture which will prepare model input, model parameters based on manipulation, analysis, and viewing of geospatial and attribute data
- Data management tool i.e. WDMULTIL
- Open model source codes which allow for improvement in the modeller community
- Integrating different modeling tools ranging from screening models to complex models for both point and diffuse sources (including PLOAD, HSPF, SWAT, AQUATOX models)
- Providing supporting tools such as model calibration (i.e. PEST), post-processing (i.e. GenScn)

The system has been developed since 1996 based on long-term service models such as HSPF (Bicknell et al., 2001), or SWAT (Arnold et al., 1994). The BASINS is widely used in the US as well as other countries (Diaz-Ramirez et al., 2008b; Jeon, 2005) due to some useful features such as linking GIS and modeling system, integrating different tools.

2.6.3. Issues of catchment water quality modeling

Catchment water quality modeling is very complex since it involves many different processes, requires substantial data as well a high level of expertise. Through a number of modeling steps, some related issues are unavoidable. Recognizing these remaining issues is very critical to understand modeling concepts as well as to improve models. In this section, four issues are discussed: (1) Model structure and model complexity; (2) scale issues; (3) ungauged catchment (limited data); (4) uncertainty

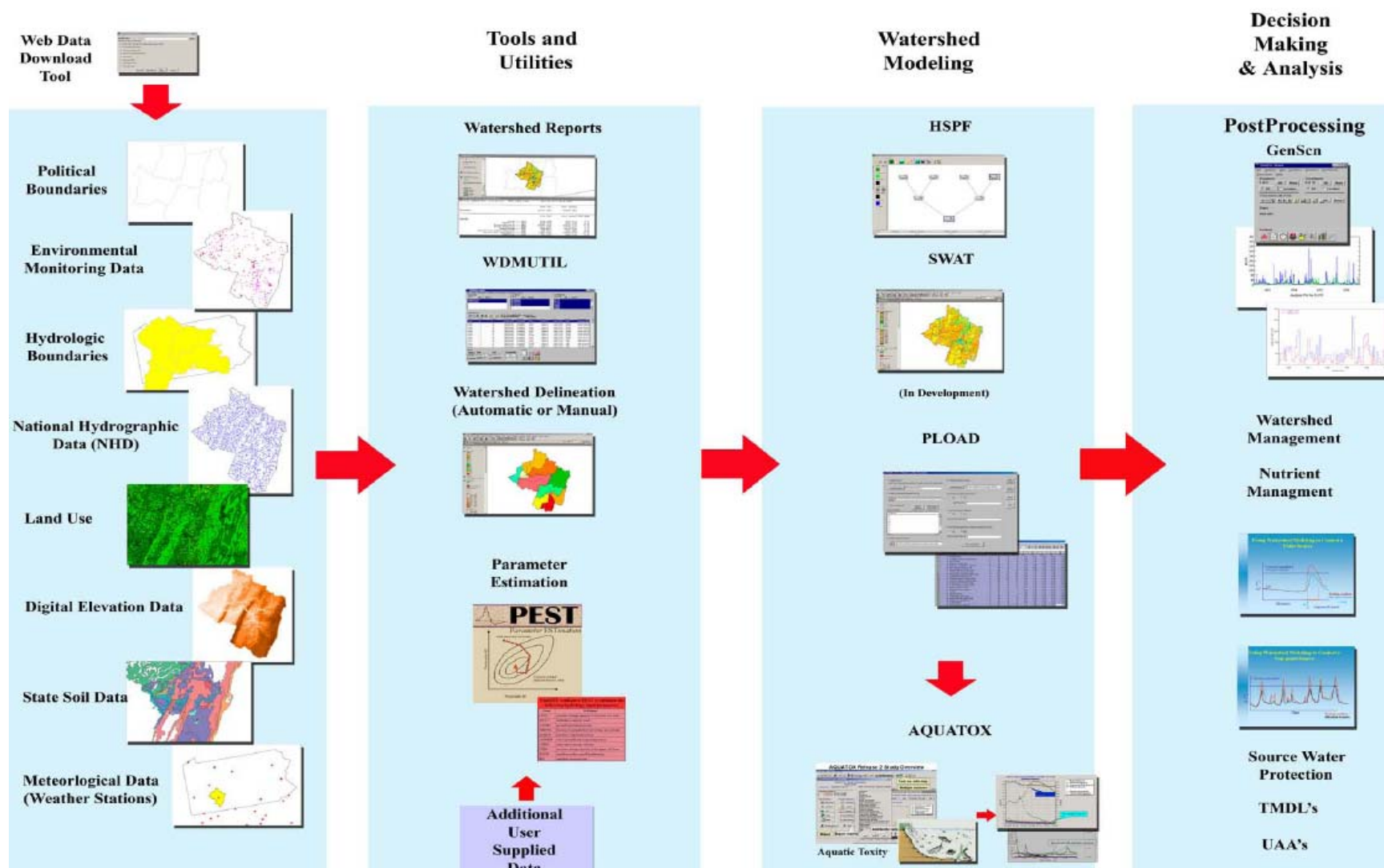


Figure 2.24: BASINS 4.0 – System overview (US EPA, 2007)

2.6.3.1. Model structure and model complexity

Model structure and model complexity accompanies each others. Model complexity is a term used to assess how complex a model structure should be evaluated. By analyzing model structure we can see how detailed the system is presented in the model. Thus, the complexity of a model is assessed by analyzing its structure. Levels of model complexity seen in literature include different groups such as (1) low, medium, or high; (2) simple, medium, or comprehensive. Loague and Green (1991) classify models according to the different levels of (i) single process, (ii) multiple processes, (iii) comprehensive, and (iv) field scale; whereas Novotny and Olem (1994) regard the diffuse pollution models as having five categories:

- Simple statistical procedures and unit loads with no interactions among the processes
- Simplified procedures with some interactions among the processes
- Simplified deterministic models, either event oriented or continuous
- Sophisticated (detailed) event simulation models
- Sophisticated continuous models

In general, model complexity increases with additional processes and mathematical algorithms introduced in the model structure, leading to three main inquiries:

- How detailed are the model domains simulated? (In term of both temporal scale and spatial scale).
- How much data or information is required to run the model?
- How does the model perform with increasing or decreasing model complexity?

The model complexity relates to how model domains are simulated (in term of both temporal scale and spatial scale). Commonly, the more comprehensive model deals with dynamic variation such as minutes or hours, whereas the simple model simulates changes annually or seasonally. The detailed model can deal with high heterogeneity of model system by means of discretization, while the simple model usually is a lumped system (Blöschl and Sivapalan, 1995). More discussions on scale issues are found in section 2.6.3.2.

Clearly, the more detailed is the model, the more data is required. In addition, more data means more time, fundings and expertises are required (McConkey et al., 2004). Thus, it is wise, when defining objectives of a specific situation, modellers have to look at data availability and anticipate specific data which can be measured during the duration of the project. However, care should be taken when dealing with decision-makers because in order to answer some specific questions from them e.g. wastewater allocation in Total Daily Maximum Load (TDML) program, a comprehensive model should be implemented. In section 2.6.3.3, “ ungauged catchment” data availability will be discussed in further detail.

McConkey et al. (2004) state the greater of complexity does not automatically increase model performance (more accurate prediction) or even bring serious problems (Schertzer and Lam, 2002, p.124). This is also found in Grayson and Blöschl (2000), Rientjes (2004) as shown in Figure 2.25, and Figure 2.26a. Model performance can easily be assessed by analyzing model error because model performance and model error are inversely related. High model performance means low errors and,

inversely, low model performance means high errors. Due to this, in literature we can see other authors relating model complexity to model error (e.g. Figure 2.26b). There is a slight difference between Figure 2.26a and Figure 2.26b. The defined optimum model performance in Figure 2.26a given certain complexity levels can be found somewhere e.g. “The model can be made no more complex than can be supported by available brains, computers and data” (Jansen, 1998, cited in De Willigen et al., 2007). In Figure 2.26b, Lindenschmidt (2005) presents a reduced model error with increasing model performance. A balance between model complexity and resources could be carefully acknowledged given the availability of data and expertise (Henderson and Bui, 2005).

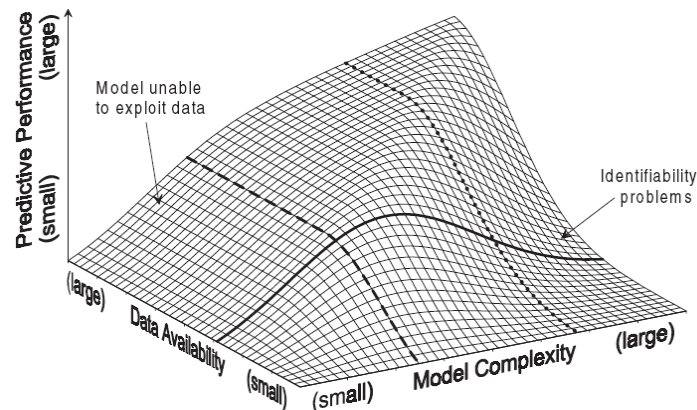
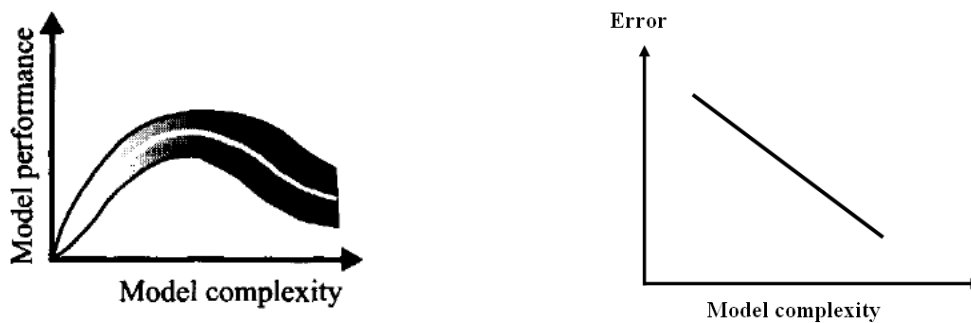


Figure 2.25: Schematic diagram of the relationship between model complexity, data availability and predictive performance. (Grayson and Blöschl, 2000)



a. Model performance and model complexity relations (Rientjes, 2004)

b. Model error versus model complexity (modified from Lindenschmidt, 2005)

Figure 2.26: Model complexity in relation with model performance and model errors

To conclude for this section, the following paragraph given by NRC (2007) can be used:

“Models are always incomplete, and efforts to make them more complete can be problematic. As features and capabilities are added to a model, the cumulative effect on model performance needs to be evaluated carefully. Increasing the complexity of models without adequate consideration can introduce more model parameters with uncertain values, and decrease the potential for a model to be transparent and accessible to users and reviewers. It is often preferable to omit capabilities that do not improve model performance substantially. Even more problematic are models that accrue substantial uncertainties because they contain more parameters than can be estimated or calibrated with available observations”.

2.6.3.2. Scale issues

Referring to the term “scale”, Blöschl and Sivapalan (1995) introduce an substantial paper in which several definitions such as observed scale; modeling scale; temporal scale; and spatial scale were mentioned. Herein this dissertation, only temporal and spatial scales are considered since they are the most applicable ones to computer-aided simulation. Examples of temporal and spatial scale are shown in Figure 2.27 where the spatial scale can range from local scale (meters) to regional scale (thousand kilometres) and the temporal scale can range from a shorter events (hours) to long term (years). Singh and Woolhiser (2002) suggest that model scales require very critical consideration during model development. Therefore, appropriate model scales must be definitely identified before starting other activities such as model algorithm development, or data measurement.

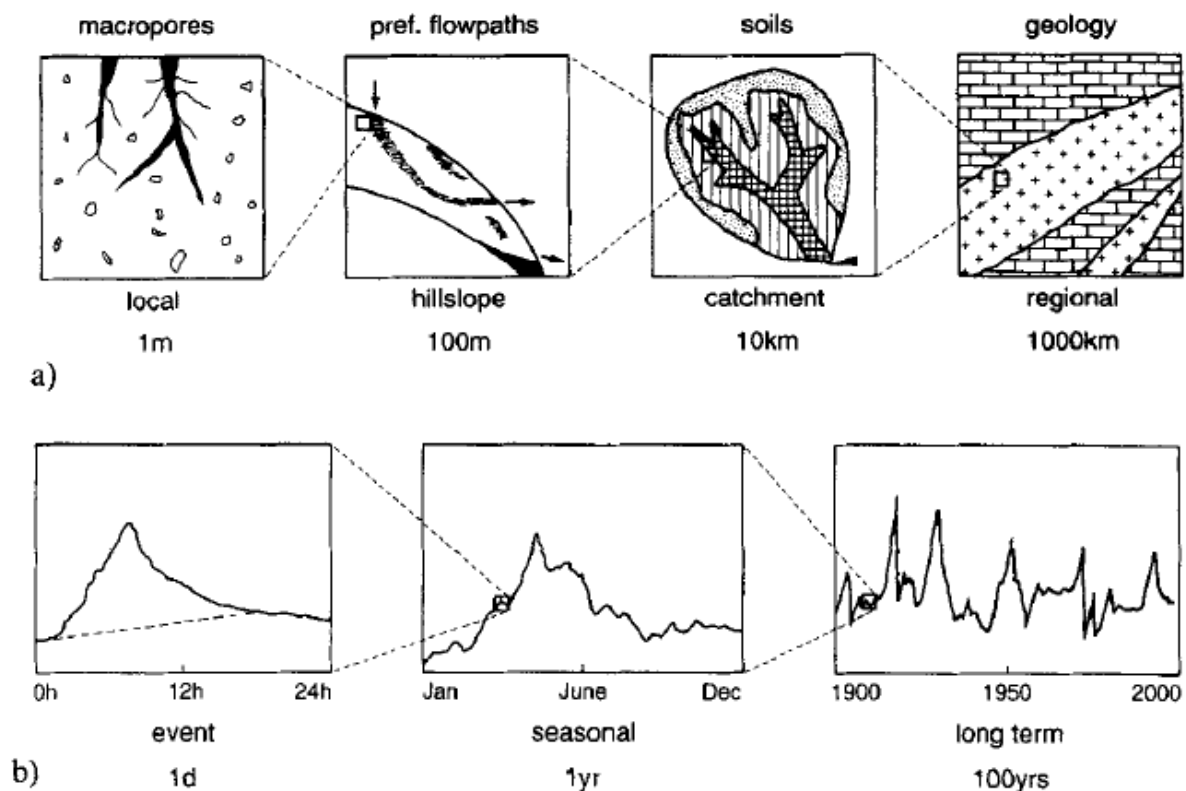


Figure 2.27: Heterogeneity (variability) of catchments and hydrological processes at a range of (a) space scales and (b) time-scales (Blöschl and Sivapalan, 1995).

Spatial scale refers to different levels of areas while the temporal scale refers to different groups of time steps. Singh and Woolhiser (2002) mention that system variables vary in space in both direction and location. Due to different factors such as discontinuities (e.g. geological structure) and various chemical and biological processes, the spatial heterogeneity of the catchment is achieved. Figure 2.28 illustrates various scales. In catchment studies, the spatial scale can vary from the local scale (such as pedon), hill slope, and catchment to regional scale. Defining these levels of scale is very important, since in the nature different processes may be dominant at certain scale and not others (Beven, 1995). Figure 2.29 and Table 2.8 are examples of scales in runoff generation processes. Different time scales are clearly illustrated. They range from minutes, hours, days (single events) to months (seasonal) and years (long term). It is interesting to note that the temporal scales relates to the spatial scales in such a

way that the smaller time step is more applicable to research at the smaller areas. By defining the spatial scale (i.e. study areas) one may be able to adopt which time scale is needed in order to fulfil research objectives as well as define a suitable data collection strategy (e.g. monitoring, archived data)

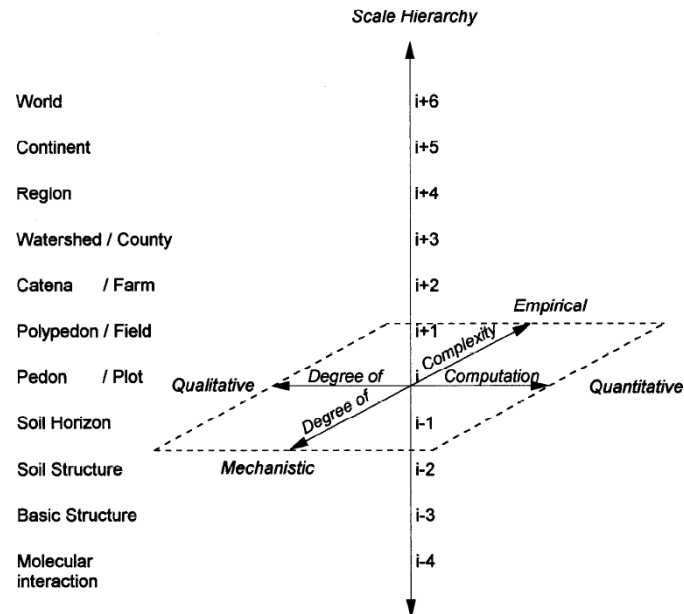


Figure 2.28: Scale hierarchy and knowledge type diagram. Model classification based on: 1) scale hierarchy, 2) degree of computation, and 3) degree of complexity (Bouma et al., 1998).

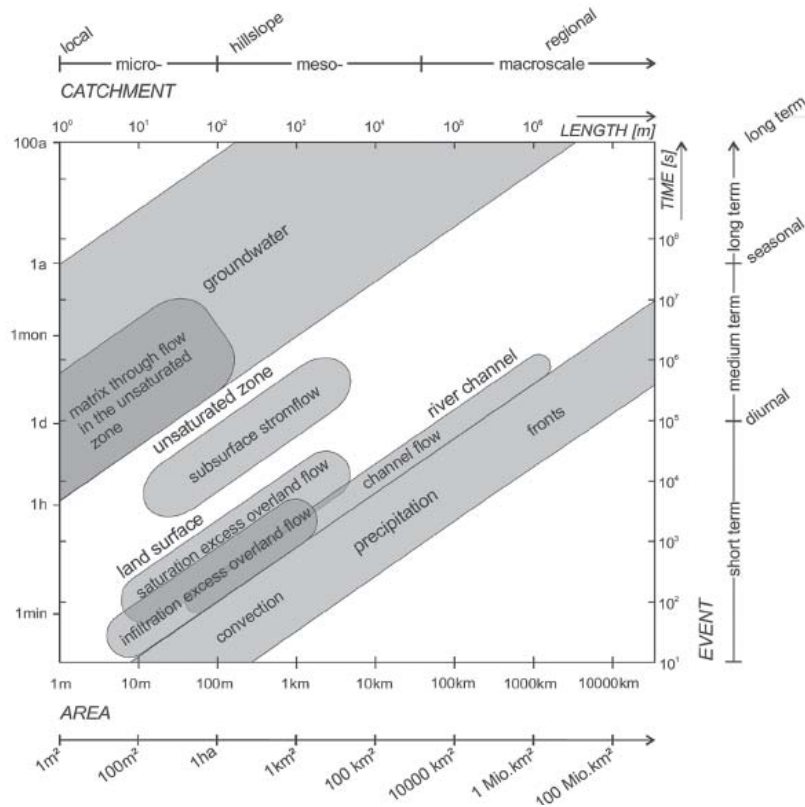


Figure 2.29: Hydrological processes at a range of characteristic space-time scales (Blöschl and Sivapalan, 1995; Bronstert et al., 2005).

The *temporal scale* is needed/used in order to capture the system variation in time. Depending on modeling objectives, simulation can be done in event (minutes/hourly times) or continuous (e.g. daily/monthly time steps) mode. The former is usually used for flood prediction and the latter is used for long-term water balance forecast.

Table 2.8: Spatial and temporal processes scales of rainfall – runoff processes (Rientjes, 2004)

Processes	Spatial scale	Temporal scale
Rainfal (convective => depression)	100 m – 100.000 m	1 min – days
Horton overlandflow	10 m – 100 m	1 min – 15min
Saturation overland flow	10 m – 1.000 m	5 min – hours
Sream flow	10 m – 100 m	1 min – hours
Unstaturated subsurface flow	1 m – 100 m	10 min – days
Perched subsurface flow	10 m – 1.000 m	10 min – 1 day
Macro pore flow	1 m – 100 m	1 min – 1 hour
Groundwater flow	10 m – 100.000 m	1 day – years
Channel flow	100 m – 10.000 m	10 min – days

Since data may not be available for the needed scale, converting information from one scale into another is needed. A technique used to accomplish such transformation is called scaling (Blöschl and Sivapalan, 1995). Detail descriptions of scaling techniques are not given here, but a part of certain methods relating to this dissertation will be mentioned (e.g. aggregation of spatial data).

Addiscott (1993) proposes questions that should be considered when translating a model from a particular scale to an appreciably larger one.

- Does the underlying hypothesis of the model remain the same?
- Do the mechanisms of the model retain their meaning in a descriptive sense?
- Is the model still being used within a range of parameter values for which it has been validated?
- Can realistic, independently-derived values still be assigned to the model's parameters?
- Is the scale of the modeling commensurate with the scale of the measurements from which the parameters were derived?
- Do the parameters at the larger scale differ appreciably from those at the smaller? If so, why?
- Has the sensitivity of the model to its parameters changed? If so, why?
- Has the classification of the model changed de facto? For example, from physically-based to lumped-parameter, or from mechanistic to functional?
- Is there anything in the use of the model at the larger scale that offends common sense?

Due to the heterogeneity of the catchment in space, spatial distribution of the system can be modelled as a lumped, semi-distributed or distributed as discussed in the model classification section 2.6.1. Existing model discretization schemes are as follows:

- Lumped scheme: The whole catchment is considered as a single spatial unit such as the SCS CN method (Ogrosky and Mockus, 1964)
- Hydrological Response Unit (HRU): the combined characteristics of land use and soil information, e.g. in SWAT model (Arnold et al., 1994)
- Land use as spatial modeling units such as in HSPF model (Bicknell et al., 2001)
- Group Response Unit (GRU): model spatial domain is subdivided into grids, and then, depending on the grid sizes, land use units belonging to the grid are grouped (Kouwen et al 1993, cited in León et al., 2001)
- A sub-catchment as a unit: A catchment is discretized into a number of sub-catchments which are later used for simulation. Typical examples of this scheme can be found in the Representative Elementary Catchment (REW) approach (Reggiani and Schellekens, 2005), HBV model (Bergstrom, 1995), CatchMODS (Newham et al., 2004)
- A catchment is discretized into equal grids; simulation is applied for each grid. This scheme is often found in physically based model e.g. SHE or SHETRAN (Abbott et al., 1986; Ewen et al., 2000)

2.6.3.3. Ungauged catchment

Data requirement is one of the greatest issues of concern in catchment modeling. The lack of data will lead to uncertain decisions, e.g. in flood prediction, or dam safety management. Hydrological data are also indispensable for enhancing knowledge of variables, hydrological processes (fluxes) and states (storage) of the hydrological system (Kundzewicz, 2007b; Peters et al., 2007). Hydrological and meteorological data collection is prerequisite in all countries. The PUB (Prediction in Ungauged Basin) initiative of the International Association of Hydrological Sciences (IAHS) looks into the reality of drainage basins and their measurement as followings, “drainage basins in many parts of the world are ungauged or poorly gauged, and in some cases existing measurement networks are declining” (Sivapalan, 2003). Thus, dealing with limited data available or in many cases “ungauged catchment,”⁷ is one of typical issue in the current hydrological community.

Data collection is lacking due to a number of reasons, mostly related to funding, and institutional aspects as well as damages during floods or other human and natural disturbances.

Techniques to deal with data limited problems can be classified into two groups:

- Regional methods: Utilizes data from gauged catchment, and then based on a similarity analysis, transfers information from a gauged catchment to an ungauged catchment. This method is close to the empirical and conceptual model and statistical aspects (see more discussions in Wagener et al., 2004).
- Geo-information techniques: Utilizes GIS data (e.g. topological parameters) and RS information (e.g. land cover, or evapotranspiration) (see Lakshmi, 2004) in order to extract relevant data for model input and model parameters. This method is very well illustrated in “*Ungauged basin analysis*” (U.S. Army Corps of Engineers, 1994).

⁷ An ungauged basin is one with inadequate records (in terms of both data quantity and quality) of hydrological observation to enable computation of hydrological variables of interest (both water quantity and quality) at appropriate spatial and temporal scales, and to the accuracy acceptable for practical application.

The “Minimum Information Requirement (MIR) concept as shown in Quinn et al.(2007), Eisele and Leibundgut (2002) can also provide an optional approach to dealing with the issue of data scarcity.

2.6.3.4. Model uncertainty

In this section, only sources of uncertainty are introduced. Other issues, e.g. uncertainty analysis will be presented in section 2.6.4.

A model is only a representation of the actual system that exists in the real world. No model can perfectly represent all of nature’s characteristics. Thus uncertainty is always a concern in the modeling process. Model uncertainty can occur at different stages of the modeling processes, e.g. model development (model complexity e.g. in Figure 2.30), data preparation (input data, parameter errors), or model calibration (validated data errors). Furthermore, different processes have different uncertainty levels as illustrated in Figure 2.31.

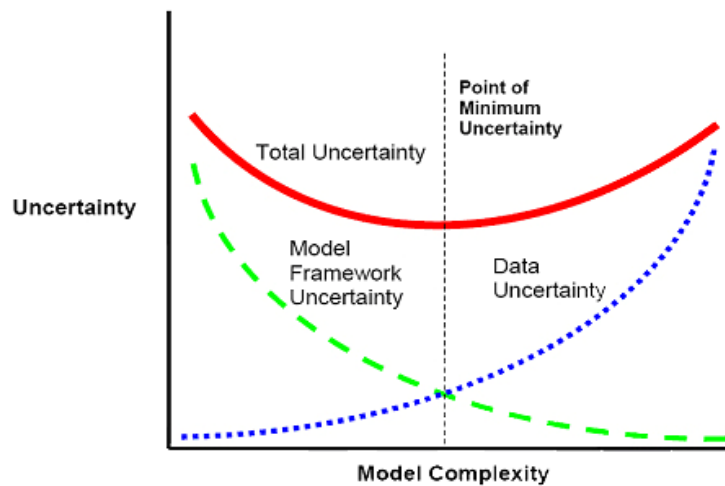


Figure 2.30: Illustration of the relationship between model framework uncertainty and data uncertainty, and the combined effect on total model uncertainty (Hanna, 1998, cited in USEPA, 2003).

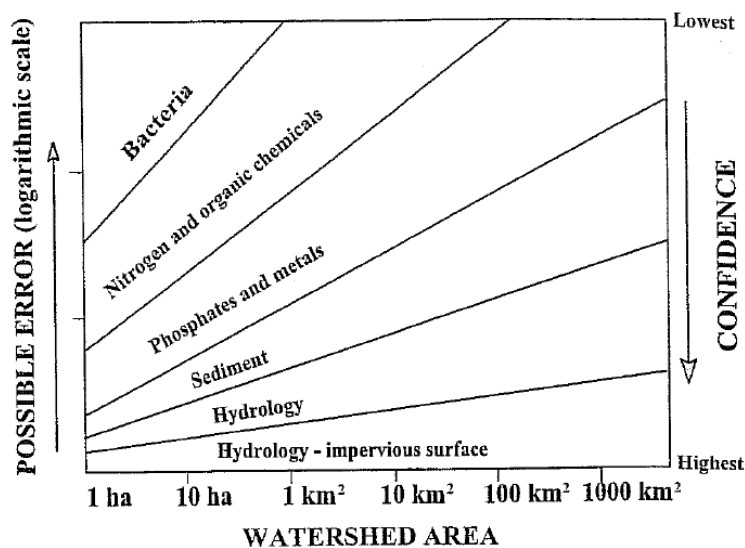


Figure 2.31: Representation of relative the accuracy of water quality modeling (Novotny, 2002).

A survey of relevant literature reveals, different sources of uncertainty typically addressed in catchment modeling such as (1) input uncertainty; (2) parameter uncertainty; (3) structure uncertainty; or (4) uncertain evaluation data (e.g. Beck, 1987; Gupta et al., 2005; Melching, 1995; Sivapalan M. et al, 2003). These four aspects are discussed as follows:

Forcing data, e.g. rainfall, is a model *input uncertainty* that is of special concern (Das, 2006; Fekete et al., 2004). The high variation of rainfall in time and space is extremely difficult to quantify. In addition, lacking of meteorological stations in developing countries will also increase the input uncertainty (Kundzewicz, 2007b; Manley and Askew, 1993). Beside the forcing data, spatial distribution data such as land cover or topography data may not be suitable for relevant field scale or catchment scale due to its low resolution as well as errors in data processing, e.g. in DEM data (Haile and Rientjes, 2005; Kenward et al., 2000).

Due to system heterogeneity as mentioned in the section “scale issues” measured parameters may not be representative of the whole model units (e.g. land use, HRU, sub-catchment). Furthermore, it is difficult to find an optimal model parameter set since different combinations of parameter sets can yield similar results (known as equifinality in Beven and Freer (2001)). This is known as *parameter uncertainty*. Model parameter uncertainty is of special concern for sub-surface parameters relating to soil properties.

Incomplete understanding of system behaviour will lead to model structure uncertainty. Relevant processes will not be well introduced into the model (Refsgaard et al., 2007). *Model structure uncertainty* can also affect model input uncertainty and model parameter uncertainty. The increase in the number of processes involved will introduce more uncertainty in model inputs and model parameters.

Uncertain evaluation data, e.g. discharge, sediment, contaminants measured at catchment outlets are often used to evaluate model behaviour. Data error due to field measurement, questionable stage-discharge curves (Hersch, 1978), and laboratory analysis are most often reported (Harmel et al., 2006a; Rode and Suhr, 2007) as mentioned in section 2.5.4.

2.6.4. Uncertainty analysis techniques

As mentioned in the previous section, uncertainty is inherent in modeling. Uncertainty analysis, therefore, has been developed to deal with this issue. Prediction of uncertainty from different sources is an aim of uncertainty analysis (i.e. input heterogeneity – input uncertainty, landscape heterogeneity – parameter uncertainty, processes heterogeneity - model structure uncertainty, Sivapalan et al., 2003) (Figure 2.32). Brown et al. (2006). Pappenberger et al. (2005), Henderson and Bui (2005) conduct comprehensive studies of uncertainty analysis techniques relating mostly to catchment modeling as well as water quality modeling. Uncertainty analysis techniques in catchment water quality modeling largely depend on data availability, i.e. evaluation data, which are used for comparison with model output. As a result, uncertainty analysis techniques are grouped into two main categories: (i) no/limited evaluation data available; and (ii) uncertainty analysis based on observed data.

When no or limited evaluation data is available, uncertainty analysis is implemented as propagating errors of the model input and model parameter through model simulations and obtaining various model outputs. Thus this technique is often defined as forward uncertainty propagation (see figure 5.15). In this approach, it is assumed that model structure is correct and approximates system characteristics (Pappenberger et al., 2005). First-order analysis or approximation (FOA) and Monte

Carlo simulation are most likely the employed methods in uncertainty propagation analysis and will be presented in next sections 2.6.4.1, 2.6.4.2.

Conditioning on uncertainty as well as model calibration based on observation data are the second next on the list of popular methods in uncertainty propagation analysis, (also termed inverse modeling, see Figure 2.33). The relationship between the model output and the observation calculated by a likelihood function is a key aspect in this approach. Parameter uncertainty can be reduced by the determination of an “optimal” parameter set or a limiting model parameter set space. Consequently, model uncertainty can also predict the best simulation output or possible ranges of variables. Three selected methods based on this approach are discussed in the next section 2.6.4.3.

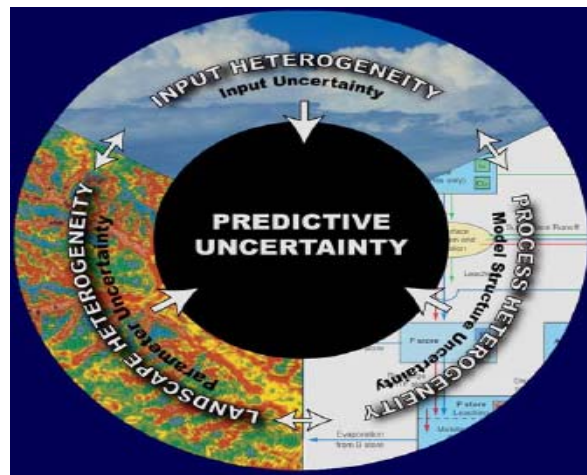


Figure 2.32: Predictive uncertainty linked with climatic and landscape heterogeneity (Sivapalan M. et al, 2003).

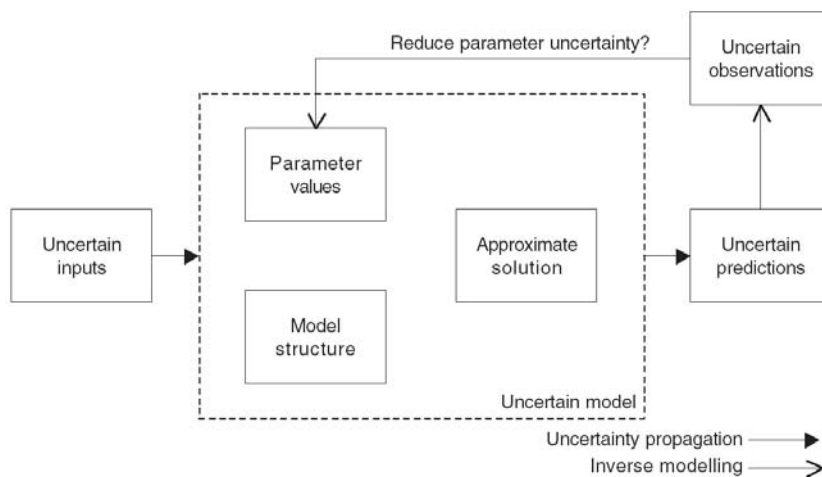


Figure 2.33: Uncertainties in model inputs combined with uncertainties in the model (parameters, structure, and solution) can propagate through the model, leading to uncertainties in model predictions. Model parameter values may be calibrated against uncertain observations through “inverse modeling.” Dependencies are not shown (Brown and Heuvelink, 2005; Brown et al., 2006).

2.6.4.1. First order Analysis

The First Order Analysis (FOA) basically relies on the Taylor series expansion. This method is sometimes known as the method of moments since it propagates and analyzes uncertainty using the first statistical moments (mean, variance), and sometimes higher order moments of the probability distribution (Morgan and Henrion, 1990). The method was popularly applied in catchment water quality modeling, especially as an uncertainty analysis tool (e.g. in Melching and Bauwens, 2001; Shen et al., 2008; Wu et al., 2006).

The method developed by Melching and Bauwens (2001) is called the Mean Value First-Order Reliability Analysis Method (MFORM) which is presented as follows:

The Taylor series expansion is truncated after the first order term:

$$C = g(X_e) + \sum_{i=1}^p (x_i - x_{ie}) \left(\frac{\partial g}{\partial x_i} \right)_{X_e} \quad (\text{eq. 2.69})$$

Where:

- C = Model output of interest
- g() = Function representing the simulation process
- X_e = Vector representing the expansion point
- p = Number of basic variables x_i

The expansion point is at the mean value of the basic variable. Thus the expected value and variance of the output are calculated approximately as:

$$E(C) \approx g(X_m) \quad (\text{eq. 2.70})$$

$$Var(C) = \sigma_c^2 \approx \sum_{i=1}^p \sum_{j=1}^p \left(\frac{\partial g}{\partial x_i} \right)_{X_m} \left(\frac{\partial g}{\partial x_j} \right)_{X_m} E[(x_i - x_{mi})(x_j - x_{mj})] \quad (\text{eq. 2.71})$$

Where:

- σ_c = Standard deviation
- X_m = Vector of mean values of basic variable

If the basic variables statistically independent, the variable of C becomes

$$Var(C) = \sigma_c^2 \approx \sum_{i=1}^p \left(\left(\frac{\partial g}{\partial x_i} \right)_{X_m} \sigma_i \right)^2 \quad (\text{eq. 2.72})$$

Where:

- σ_i = Standard deviation of the basic variable i

An advantage of the FOA is that it required only the first two statistical moments of input distribution. However, it yields only this moment for output distribution. In addition, the FOA assumes model linearity which is not often the case in comprehensive models. Thus, this method is commonly used as a supporting method in differential sensitivity analysis (Morgan and Henrion, 1990, p.213). The accompanying method is, for example, the Monte Carlo simulation for uncertainty analysis.

2.6.4.2. Monte Carlo simulation

Monte Carlo simulation technique involves random sampling of model input and/or model parameters to produce hundreds or thousands of scenarios, i.e. outputs (see Vose, 1996). The model results are stored and then evaluated statistically. In this way, uncertainty in model input and/or model parameters which are presented as probability distributions will propagate through simulation systems. Therefore, uncertainty in model results can be explicitly observed. Figure 2.34 shows an example of implementing the Monte Carlo simulation in water quality modeling. Here, random numbers of model parameters are generated from a suitable program then applied through a deterministic model. This process is repeated many times to produce a corresponding output which are analyzed statistically (Novotny, 2002).

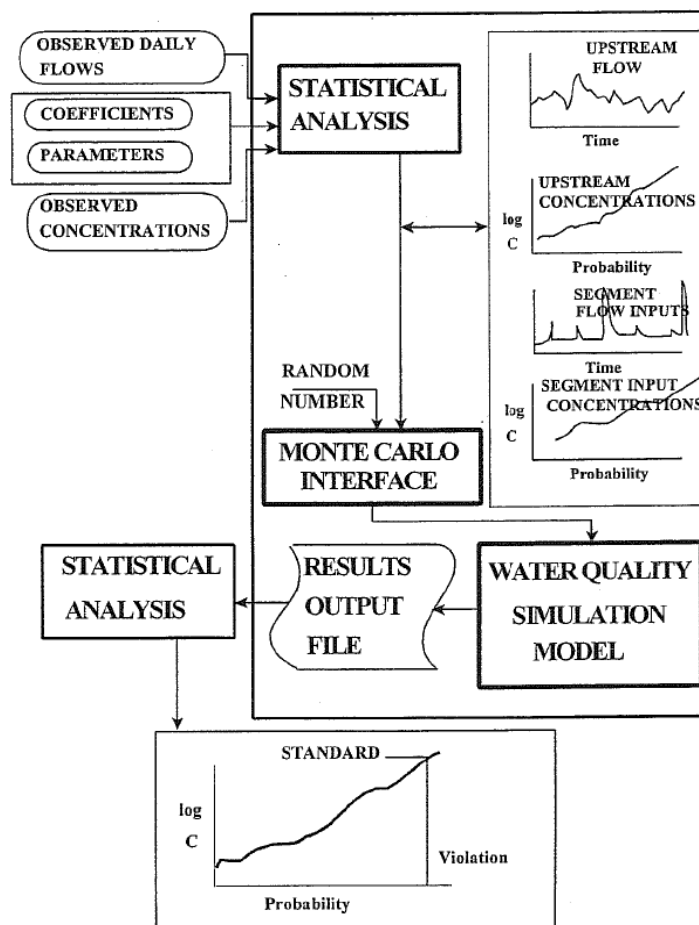


Figure 2.34: Monte Carlo modeling schematic (Novotny, 2002)

Two important aspects of the Monte Carlo simulation are the sampling technique and the analysis of model output.

Sampling technique refers to a method to generate random numbers given the probability distributions. Several sampling schemes have been developed, e.g. normal sampling (crude Monte Carlo sampling), or Latin Hypercube sampling. Latin Hypercube is the most often implemented scheme in statistical packages in numerous applications (e.g. in Melching and Bauwens, 2001; Shen et al., 2008; Wu et al., 2006). A stratified sampling using Latin Hypercube is different from the Monte Carlo sampling in terms of equal probability distribution in the probability distribution as shown in Figure 2.35.

Analysis of model output is mostly to obtain a confidence range of simulated results. As an example, the method given by Morgan and Henrion (1990) is explained. The series of model output (e.g. m results) are rearranged and labelled as in increasing order.

$$y_1 \leq y_2 \leq \dots \leq y_m$$

y_i is an estimate of fractile Y_p , where $p=i/m$

Let (y_i, y_k) is a pair of sample values constitutes a confidence interval with confidence α

Where:

- y_i = Estimate of $Y_{p-\Delta p}$
- y_k = Estimate of $Y_{p+\Delta p}$
- i = $\left(mp - c\sqrt{mp(1-p)} \right)$, rounding down
- k = $\left(mp + c\sqrt{mp(1-p)} \right)$, rounding up
- c = Deviation enclosing probability α of the unit normal
i.e. $P(-c < \phi < c) = \alpha$

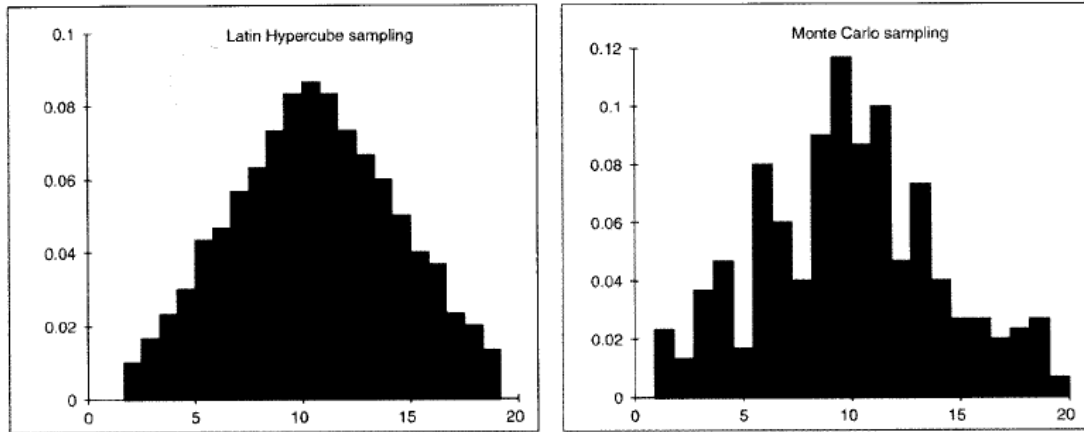


Figure 2.35: Comparison of probability distributions between Latin Hypercube (left) and Monte Carlo (right) (Vose, 1996).

As pointed out by Dilks et al. (1992), one major limitation of the Monte Carlo simulation is the limited data on model parameters that leads to inadequate estimation of probability distribution. Therefore, estimating parameters using observation is suitable to compensate for this method.

2.6.4.3. Parameter optimization and sensitivity analysis (model calibration)

Parameter optimization is one way to reduce uncertainty caused by improper model parameters. Parameter calibration is a process for which model output is adjusted by “optimizing” model parameters in order to match observation data, e.g. see Figure 2.36. The state of the art optimization techniques in catchment modeling can be seen in the work by Duan et al.(2003) and Sorooshian and Gupta (1995).

Model parameters include physical parameters and process parameters. “Physical” parameters which represent physically measurable catchment properties such as area, slope, shape, etc. can be estimated or calculated from topographic maps and field surveys. These parameters are usually fixed during modeling processes. “Process” parameters represent catchment properties that are not directly

measurable such as the curve number (CN), or the “effective” depth of surface soil moisture storage. These parameters are calibrated through model optimization (Sorooshian and Gupta, 1995).

Model calibration can be implemented either manually or automatically. Manual calibration is just a “trial and errors” process. Given initial values, e.g. from literature, parameters are changed manually until model outputs approach observation, i.e. evaluation based on visual comparison or criteria⁸. Manual calibration requires a certain level of expertise, therefore, manual calibration can cause frustration to inexperienced and untrained person because of its, tedious and time consuming nature (Sorooshian and Gupta, 1995; Van Griensven, 2002).

Given the development of computing science, automatic calibration has been increasingly implemented in modeling packages or as independent sharewares. The automatic calibration procedure typically includes four important components. Those are: (1) objective function(s), (2) optimization algorithms, (3) termination criteria, and (4) calibration data. These four components are greatly discussed in Sorooshian and Gupta (1995). The first component, the objective function, is basically a comparison function between simulated and observed data, e.g. streamflow. Popular functions are Nash-Sutcliffe Efficiency, Weighted Least Square (WLS), Maximum Likelihood (see more in Van Griensven, 2002). The second component, optimization algorithm, is the most difficult to work with since existing parameter combinations have similar results, e.g. lacking of identifiability or equifinality (Beven and Freer, 2001). Searching techniques to meet optimal parameters are currently still an area for the researchers to exploit (Duan et al., 1993). The methods include local and global search in “response surfaces,” i.e. parameter spaces defined by objective functions. However, recommended by Sorooshian and Gupta (1995), among various algorithms, the Shuffled Complex Evolution (SCE-UA), a global optimization method, developed at the University of Arizona (Duan et al., 1993) is the best method available for parameter estimation of conceptual catchment model. The termination criteria are applied so that the searching is stopped during the iterative loops when the most appropriate convergence function of the parameters has been reached. The quality of calibration data will be included in section 2.6.4.3.

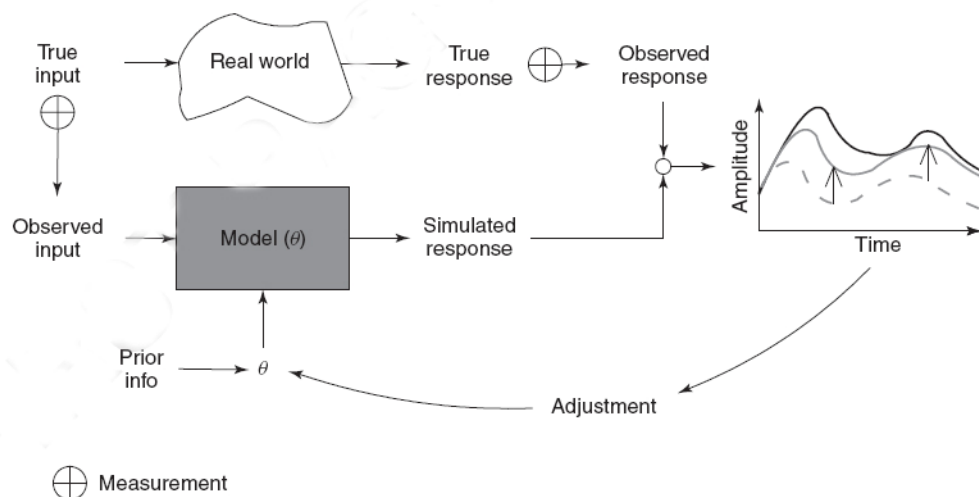


Figure 2.36: Strategy for model calibration. The model parameter set is represented by θ (Gupta et al., 2005)

⁸ model criteria are presented in section 2.6.5.4

Another important aspect in model calibration is to define which parameters to use for optimization, especially when dealing with complex models. A method to do this is called “**sensitivity analysis**”. By manually or automatically changing model parameters, the variations of model output can be observed. The most sensitive parameters are the ones affecting model output the most that is recorded for model calibration. Sensitivity analysis techniques can be found in Saltelli et al. (2004).

Although model calibration is still a common practice in modeling, an “optimal” parameter set does not seem to exist in the real world. Different combinations of model parameters can yield similar model results. This is termed as “equifinality” as mentioned in (Beven and Freer, 2001; Beven and Binley, 1992). Typical reason for this issue could be the effect of aggregated processes (temporal and spatial). Constant parameters can not be representative across scales (Stow et al., 2007). Therefore, as recommended by Stow et al. (2007), “the perspective of water quality modellers should change from seeking a single “optimal” value for each model parameter, to seeking a distribution of parameter sets that all meet a pre-defined fitting criterion” Following this perspective, the Bayesian inference framework is a good choice.

Bayesian inference

Bayesian inference is another technique to account for parameter uncertainty based on observation data. The model parameters that yield the observed data are calculated in terms of a probability distribution based on Bayesian’ theorem as in the following equation:

$$p(\theta|Y) = \frac{p(Y|\theta)p(\theta)}{p(Y)} \quad (\text{eq. 2.73})$$

Where:

- θ = Model parameter
- $p(\theta)$ = The prior distribution
- $p(Y|\theta)$ = “probability of data y given θ ” or likelihood function (as a function of θ), this is derived from a joint probability function: $p(\theta, Y) = p(\theta)p(Y|\theta)$
- $p(\theta|Y)$ = The posterior distribution
- $p(Y)$ = Marginal distribution of Y $\sum_{\theta} p(\theta)p(y|\theta)$ and the sum is over all possible values of θ

Or $p(Y) = \int p(\theta)p(y|\theta)d\theta$ in case of continuous θ .

In Bayesian inference, model parameters are considered random variables, thus, they are associated with a certain probability. Therefore, defining *the prior distribution* $p(\theta)$ for a parameter is rather subjective. Basically, there are three types of prior distributions, namely informative, non-informative and conjugate distribution. The informative prior is defined given a standard probability distribution of the prior. Non-informative prior means no information is available. In this case, usually the uniform distribution is chosen. The conjugate prior distribution is implied if the prior is chosen from a probability family and the posterior is also a member of this family.

Based on this theorem, any quantity of *the posterior* can be calculated, e.g. moment, quantiles, or highest posterior density region. These quantities can be expressed in terms of posterior expectation of θ . The posterior expectation of a function $f(\theta)$ is (Gilks et al., 1996a)

$$E[f(\theta)|Y] = \frac{\int f(\theta)p(\theta)p(Y|\theta)d\theta}{\int p(\theta)p(Y|\theta)d\theta} \quad (\text{eq. 2.74})$$

The interaction in this expression is difficult in practice, especially when dealing with complex models. The Markov Chain Monte Carlo algorithm offers a solution for this equation (e.g. see in Gilks et al., 1996b; Kuczera and Parent, 1998; Stow et al., 2007).

The likelihood function $L(\theta), P(Y|\theta)$

It should be noted that the likelihood function is a special case of the objective function presented in previous section “model optimization.” The *objective function (OF)* is to measure quantitatively the fitness between model results and the observed data. The function **may or may not have a probabilistic basis**, while the *likelihood function* is a function measuring the probability of a given data set (see in McIntyre, 2004).

Assuming the simulation errors follow the normal distribution:

$$Y = f(I, \theta) + \varepsilon \quad (\text{eq. 2.75})$$

Where:

$$\begin{aligned} Y &= \text{Observations} \\ f(I, \theta) &= \text{Model functions with } I \text{ (input), } \theta \text{ (parameters)} \\ \varepsilon &= \text{Simulation errors (residuals),} \end{aligned}$$

The likelihood function for n observations assuming residuals are mutually independent, identically and normally distributed, $N(0, \sigma^2)$ is:

$$L(\theta) = \frac{1}{(\sqrt{2\pi})^n \sigma^n} \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^n (Y_i - Q_i)^2\right) \quad (\text{eq. 2.76})$$

Where:

$$\sigma^2 = \text{Model variance (mean squared difference between predicted and observed values)}$$

The marginal distribution $p(Y)$

This is also known as the prior predictive distribution. “Prior” because it does not depend on a previous observation; “predictive” because it is the distribution of a observable quantity (Gelman et al., 2004). The $p(Y)$ represents the joint likelihood of the data and the parameters and will be constant for all values of θ . Thus, the Bayesian’s theorem can be rewritten as:

$$p(\theta|Y) = c \times p(Y|\theta)p(\theta) \text{ or } p(\theta|Y) \propto p(Y|\theta)p(\theta) \quad (\text{eq. 2.77})$$

Where:

$$c = \text{Normalizing constant}$$

A significant feature in Bayesian inference is the ability to update data sequentially. The posterior becomes prior when the new data is available (see Figure 2.37). Bayesian inference is recommended for adaptive water management⁹ because of this feature (e.g. NRC, 2001; Stow et al., 2007).

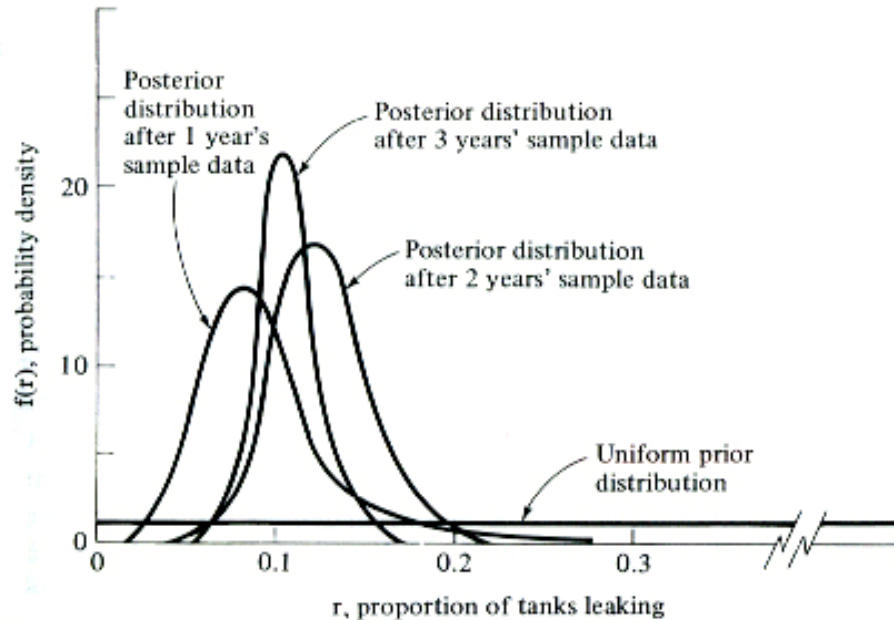


Figure 2.37: An example of prior and posterior distribution in Bayesian estimation of a parameter (applicable to underground tanks that are lacking in a large population based on annual sample data) (Morgan and Henrion, 1990, p.85).

The Bayesian inference is now popular in different fields, as is catchment water quality modeling (e.g. Borsuk et al., 2002; e.g. Dilks et al., 1992; Engeland et al., 2005; Qian and Reckhow, 2007). The essential steps in using a Bayesian approach are to (Todini, 2007):

- Define a subjective prior density for the parameters
- Assume an appropriate likelihood for the parameters namely a probability density of observation given parameters coherent with the Bayes theorem
- Derive a pdf for the parameter from the observation (the posterior density)
- Compute the probability density of the predictand conditional on the parameters
- Marginalise the parameter uncertainty by integrating, over the parameter space, the derived parameters posterior pdf times the probability density of the predictand conditional upon the parameters

There are several approaches in implementing the Bayesian inferences, e.g. Bayesian Monte Carlo (Dilks et al., 1992), Markov Chain Monte Carlo (Kuczera and Parent, 1998), Generalized Likelihood Uncertainty Estimation (GLUE) (Beven and Binley, 1992). Comparisons of these methods can be found in literature (e.g. in Qian et al., 2003; Stow et al., 2007). Hereunder, the two most common methods are presented, namely the Generalized Likelihood Uncertainty Estimation (GLUE) and the Markov Chain Monte Carlo.

⁹ The adaptive water management will be mentioned in chapter 6.

Generalized Likelihood Uncertainty Estimation (GLUE)

Based on the Bayesian inference framework, Beven and Binley (1992) introduce the Generalized Likelihood Uncertainty Estimation (GLUE) making possible the parameter data sets equifinality (non-uniqueness, non-identifiability). This approach is widely applied in environmental modeling as listed in Balin (2004), e.g. hydraulic applications, erosion modeling, groundwater modeling, land-surface atmosphere modeling, atmospheric deposition, regionalization studies, flood frequency modeling, rainfall modeling and runoff-rainfall modeling

The steps in the GLUE methodology are as follows (Gupta et al., 2005):

- Decide on a model structure or structures to be used.
- Sample multiple sets of values from prior ranges or distributions of the unknown parameters by Monte Carlo sampling, ensuring independence of each sample in the model space. (i.e. important sampling (Balin, 2004))
- Evaluate each model run by comparing observed and predicted variables.
- Calculate a likelihood measure or measures for those models considered behavioural.
- Rescale the cumulative likelihood weights over all behavioural models to unity.
- Use all the behavioural models in prediction, with the output variables being weighted by the associated rescaled likelihood weight to form a cumulative distribution of predictions, from which any desired prediction quantiles can be extracted.

One of the most interesting aspects in the GLUE approach is the likelihood function. Recognizing the difficulties of the Bayesian inference, e.g. difficulty in defining a likelihood function, the complexity of response surface due to model error interaction, the GLUE approach uses pre-defined likelihood functions (Table 2.9). By using these subjective likelihood measures, the whole response surface are explored so that many different combinations can be accepted (Engeland et al., 2005). However, the likelihood function in GLUE is recently criticized by Mantovan and Todini (2006) and Todini (2007). They argued that the GLUE likelihood functions, those in table 5.2, are not formal enough (Beven, 2009; Mantovan and Todini, 2006; Todini, 2007). This consequently will reduce information that can be extracted from observed data. Therefore, proceed with the GLUE method with care.

Table 2.9: Example of likelihood measures for GLUE methodology (Beven and Freer, 2001).

Likelihood measures	Descriptions
Autocorrelated Gaussian error model	$L[Z_T \theta, \Phi, Y_T] = (2\pi\sigma^2)^{-T/2} (1-\alpha^2)^{1/2} \exp\left[-\left(\frac{1}{2\alpha^2}\right)\left\{(1-\alpha^2)(\varepsilon_1 - \mu)^2 + \sum_{t=2}^T (\varepsilon_t - \mu - \alpha(\varepsilon_{t-1} - \mu))^2\right\}\right]$
Inverse error variance	$L[M(\theta Y_T, Z_T)] = (\sigma_e^2)^{-N}$
Nash and Sutcliffe criterion	$L[M(\theta Y_T, Z_T)] = (1 - \sigma_e^2 / \sigma_o^2)^{-N}, \sigma_e^2 < \sigma_o^2$
Exponential transformation of error variance	$L[M(\theta Y_T, Z_T)] = \exp(-N\sigma_e^2)$

σ_e^2 and σ_o^2 are the error variance and the variance of observation, $M(\theta|Y_T, Z_T)$ indicates the i^{th} model conditioned on input data Y_T and observation Z_T , $\Phi(\mu, \sigma, \alpha)$ is the error parameter, and τ is number of time steps in the simulation

In addition, the prediction quantiles $P(\hat{Z} < z)$ in GLUE is calculated as:

$$P(\hat{Z} < z) = \sum_{i=1}^B L \left[M(\theta) \left| \hat{Z}_{t,i} \right. \right]$$

Where:

$$\hat{Z} = \text{Value of variable } z \text{ at time } t \text{ by model } M(\theta)$$

This quantile relates to the predicted variable \hat{Z} , not to observation data. This will result in “*extremely flat*” *posterior probability distribution*” (Todini, 2007). Moreover, Balin (2004) points out that GLUE is limited in complex modeling since the concept requires a huge number of experimental trials.

Despite its limitations, the GLUE approach is still popular in current modeling practice because of several advantages e.g. *easy-to-use, single ready-made package, and simple understandable ideas* (Mantovan and Todini (2006)). Moreover, the “equifinality” that can be explored in GLUE are still quite reasonable (Romanowicz and Beven, 2004; Todini, 2007).

Markov Chain Monte Carlo

As pointed out in previous section, the limitations of the GLUE approach are (1) sampling directly from prior distribution, and (2) the subjective likelihood. Since the prior is usually defined as a uniform distribution, the posterior mainly depends on the likelihood function that leads to the method based on likelihood only, thus, Bayesian inference is not fully utilized. The Markov Chain Monte Carlo (MCMC) approach is an option to fulfil this gap.

By implementing the MCMC method, the Bayesian theorem can easily be solved numerically in an accurate manner (Gelman et al., 2004; Gilks et al., 1996b), especially when dealing with numerical integration for sampling in high-dimensional distribution. The MCMC method samples directly from posterior in order to cover the possible probable region of, $p(\theta|Y)$ which is not easily done with sampling from the prior. The innovative idea behind the MCMC is to create a Markov process and run the process long enough so that the resulting sample closely approximates a sample from $p(\theta|Y)$ (See more discussions in Qian et al., 2003).

Implementation of the MCMC requires two steps (Balin, 2004):

- Choice of simulation error modeling strategy
- Choice of sampling strategy to estimate model parameter.

The simulation error is often modelled using the likelihood function, while Metropolis algorithm is the best choice for sampling strategy. Expression of this likelihood function using normal distribution is as follows:

$$L(\theta) = \frac{1}{(\sqrt{2\pi})^n \sigma^n} \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^n (Y_i - Q_i)^2\right) \quad (\text{eq. 2.73})$$

The Metropolis algorithm includes three steps: (1) generation of new samples from previous generated samples, (2) acceptance of the new generated parameter set, and (3) monitoring the convergence of the algorithm. Detail mathematical expressions for this algorithm can be found in standard texts (e.g. Gelman et al., 2004; e.g. Gilks et al., 1996b), so it is omitted here.

In this “uncertainty analysis” section, most popular methods used in catchment modeling have been presented. These methods can basically deal with problems of input uncertainty and parameter uncertainty. Model structure uncertainty analysis is not mentioned yet due to e.g. assuming that typical environmental processes are well presented. In order to confirm this assumption, re-accessing model performance in many different aspects should be required. Once inconsistency in model output is observed, it is time to re-design the modeling framework and continue to test the model. Therefore, the analysis model structure can be regarded as an interactive process and will take a long time. Some publications on this topic can be found in literature (e.g. in Gupta et al., 2005; Refsgaard et al., 2007; Wagener and Gupta, 2005).

2.6.5. Model selection

2.6.5.1. Review model projects

In order to understand the processes of source formations, transformations and transportations as well as controlling pollution, mathematical models are regarded as powerful tools to aid in such understanding (e.g. Singh and Woolhiser, 2002). Catchment models are fundamental to water resources assessment, development, and management. They can be used to analyze the quantity and quality of stream flow, reservoir system operations, groundwater development and protection, surface water and groundwater management, water distributed systems, water use, and a range of water resources management activities. In addition, catchment models are employed to better understand the dynamic interactions between climate and land-surface hydrology (Wurbs, 1994). Borah and Bera (2004) state that understanding and evaluating the natural processes in a catchment lead to impairments, and problems are continuing challenges for scientific and engineers. Mathematical models simulating these complex processes are useful analysis tools to understand the problems and to find solutions through land-use changes and best management practices (BMPs). Horn et al. (2004) mention the use of modeling tools to evaluate river quality and to assess management practice for the improvement of aquatic health and function, e.g. in EU Water Framework Directive and the US TDML. However, given the fact that numerous models are available, determination and adoption of a suitable model is still a difficult concept to apply. Hereunder are typical projects in which model review or selection was an essential step.

European projects

The River Basin Management Plans (RBMP) under the WFD, EUROHARP project (Schoumans and Silgram, 2003) explains 15 aspects of a catchment water-quality tool, and reviews 9 quantification tools from simple to complex (e.g. from static to dynamic) in great detail. In addition, in order to evaluate a model, they suggest several important topics *for scientific evaluation* such as: (1) spatial and temporal resolution, (2) pathways represented, (3) process and nutrient species considered; and *for operational evaluation* include: (1) potential costs of application, (2) restrictions for applications (scenario analyses) and (3) applicability. These topics are used to compare with the 9 quantification

tools which have mostly been developed in Europe except SWAT. They are NL-CAT, MONERIS, REALTA, TRK (SOILNDB/HBV-N), SWAT, EveNFlow. The review demonstrates that the EUROHARP quantification tools differ profoundly in their approach to predict the diffuse nutrient losses from agricultural land to surface freshwater systems. This is a reflection of differences in (i) their level of complexity, (ii) their representation of system processes and pathways, and (iii) their resource (data and time) requirements. The quantification tools range from complex to process-based models.

Benchmark Models for the Water Framework Directive

The Benchmark (BMW) projects (Benchmark Models for the Water Framework Directive) (Boorman et al., 2007; Kämäri et al., 2006; Saloranta et al., 2003) provide advice and criteria selection of the use and evaluation of models to aid the implementation of the Water Framework Directive (WFD) in order to answer the question: “What type of models should be the most suitable for use in the context of the WFD?”. The most notable results from this project were a model selection protocol (Boorman et al., 2007), benchmark criteria and scoring scheme (Kämäri et al., 2006; Saloranta et al., 2003) etc. which are very helpful for model selection (see appendix 1). Arheimer and Olsson (2003) compile the most current water-quality models (37 models) used in Europe, in which 9 catchment water-quality models were often cited (e.g. MIKE-SHE, SWAT, HBV, AGNPS). This evaluation is useful to a water manager in deciding what model(s) to apply in a particular case.

USA projects

The Total Daily Maximum Load (TDML) is the most comprehensive program carried out in the US in order to improve the water quality. Several measures have been taken to compile and evaluate the water quality models that are available. A series of work conducted by Shoemaker and co-workers include: Compendium of Catchment-Scale Models for TMDL Development (Shoemaker et al., 1992); Compendium of Tools for Catchment Assessment and TMDL Development (Shoemaker et al., 1997); TMDL Model Evaluation and Research Needs (Shoemaker et al., 2005). In these works, a number of models were evaluated with intent to develop a TDML project. Catchment water quality model was employed as the catchment-scale loading model in these reviews. More than 20 models were analyzed according to their features and capacities. The models were also compared on the basis of complexity, capabilities and interface characteristics. A recent review by Borah et al. (2006) present a number of sediment and nutrient models which can utilize in TDML. The review included a wide range of simulation tools. They (Borah et al., 2006) also pointed out current model limits and potential, and ways to improve for future TDML implementations (e.g. combining advantages aspects of each model) (Borah et al., 2006). Parson et al. (2004) conduct a comprehensive review of agricultural non-point source water quality models. This review provides model developments for catchment water quality modeling within the last few decades. The review also includes a description and evaluation of 12 models.

Borah and Bera (2003) conduct an extensive review of catchment water quality models for both event (e.g. AGNPS, ANSWERS, DWSM, KINEROS) and continuous (e.g. AnnAGNPS; ANSWERS-Continuous, HSPF, SWAT, MIKE-SHE) simulations. They focus on model capability, temporal and spatial representation, mathematical strength, and applicability of hydrology, sediment, chemical, and BMP components. In their conclusion, DWSM is most suitable for the event simulation, and HSPF and SWAT are best fitted for the continuous one.

In these reviews, the most recent catchment water quality models developed by the US and Europe institutions have been considered. Though the detailed description of each work is different from others, the main goal was to help modellers and water manager select the model approach that is most suitable to a particular purpose.

2.6.5.2. Model selection consideration

Based on extensive reviews of available model selection projects as described above, review papers (Borah and Bera, 2003; Borah et al., 2006; e.g. in Loague and Green, 1991; Merrit et al., 2003; Singh and Woolhiser, 2002) as well as a comprehensive discussion from the beginning of this chapter, a criteria or aspects for the model selection for catchment water quality simulation are presented in Table 2.10. The criteria are taken into account for the model selection and development described in chapter 4 and chapter 5.

Schoumans and Silgram (2003) emphasize model selection as “the final selection of a particular model for particular catchment will depend on the question being asked, the data availability, the resource limitations, and the physical characteristics of the catchment in questions (with limit the suitability of some models)”. In this thesis, a strategy for selecting a model among various model is carried out. Eight often-cited models are analyzed including two empirical model (ANGPS, CNS), four conceptual model (SWAT, HSPF, HBV, ANSWER-2000), and two physically –based model: (SHE and SHETRAN, DWSM)

Table A1.4 in appendix 1 provides a summary of eight analyzed catchment water quality models. The models are selected based on following criteria:

- The most often cited models in literature
- Detail description for each model is available
- State of the art of each model (other models such as SWRRB, EPIC, CREAMS, GLEAMS had been incorporated in SWAT (Arnold and Fohrer, 2005))

Ability to simulate nutrient (nitrogen and phosphorus) dynamics (other model such as TOPMODEL (Beven et al., 1995), KINEROS (Woolhiser et al., 1990), WEPP (Flanagan and Nearing, 1995) is limited only to hydrology, erosion components.

Table 2.10: Model selection aspects and description considered for selection and development of catchment nutrient modeling in this study

ID	Aspects	Description
1	What are the dominant system processes?	<p>Prior analysis system complexity in order to adopt suitable model structures, e.g. according to practical conditions. (Assumptions on underlying processes can be implied)</p> <p>+ Hydrology (e.g. Horton overland flow, saturated overland flow, groundwater flow)</p> <p>+ Erosion and sedimentation processes (e.g. soil detachment and transportation)</p> <p>+ Nutrient transformation in soil and water</p> <p>+ Nutrient transportation</p>

ID	Aspects	Description
2	How to discretize system domains?	+ Presentation of the catchment as well as variable dynamics in time + Spatial (e.g. lumped, distributed) + Temporal (e.g. event or continuous, minutes/hourly or daily/monthly)
3	Which modeling approach is applicable?	Focus on scientific bases of mathematical expressions + Empirical model + Conceptual model + Physically-based model
4	What are the available data?	Data availability and potentiality + Archived data (e.g. Geo-information, meteorology) + Monitored data (e.g. discharge, water quality)
5	What are sources of uncertainty and <i>uncertainty analysis techniques</i> ?	Assessing related errors in model + Input data + System complexity (model parameter, model structure errors) + Accompanying uncertainty analysis technique
6	Is the approach suitable for practical use?	Focus on expertise requirements + Requests from government + Robust/Practical/Operational + Input/Output visualization

A scoring scheme for selecting the most suitable implementing model has been developed based on the review of eight models and their selection issues. The scheme ranges from 0 to 3 for each criterion. The model which gets the highest score after summation is judged to be the most suitable. Results based on this scoring scheme are presented in Table 2.11. The HSPF model is chosen for having the highest score and will be briefly presented in next section.

1) Model structure

- 0: not included in model
- 1: empirical approach
- 2: conceptual approach
- 3 : physically-based approach

(2) Model scale

- 0: monthly or longer, catchment is lumped as 1
- 1: daily or longer, semi-distributed model
- 2: hourly or longer, semi-distributed model
- 3: hourly or longer, distributed model

(3) Data requirement

- 0: too many data required

- 1: many data
- 2: many data, detailed instructions on data collection i.e. user manual
- 3: few data required

(4) Model objective: to simulate nutrient dynamics during flood events at catchment scale induced by both point and diffuses sources

- 0: can not implemented
- 1: a lot of improvements of original model are required i.e. improve model algorithms
- 2: a certain improvements of original model are required
- 3: directly utilized as provided

(5) Model instructions clearly depend on available resources.

Table 2.11: Scoring table by the auhor for 8 models listed in appendix 1

Criteria	AGNPS	CNS	SWAT	HSPF	HBV	ANSWERS -2000	SHE and SHETRAN	DWSM
1. Model structure								
Hydrology	1	1	2	2	2	2	3	3
Erosion and sedimentation	1	0	2	2	2	2	3	3
Nutrient	2	2	3	3	3	3	3	2
River routing	1	0	2	2	2	2	3	2
2. Scale								
Temporal discretization	1	0	3	3	2	3	3	3
Spatial discretization	1	1	3	3	2	3	3	2
3. Data requirement								
Input data	3	3	1	2	2	2	1	2
Model parameters	3	3	2	2	2	2	1	2
4. Modeling objectives	2	0	2	3	2	2	2	2
5. Model instructions	3	2	3	3	2	2	1	1
Sum	18	12	23	25	21	23	23	22

2.6.5.3. Selected model - the Hydrological Simulation Program – FORTRAN (HSPF)

The Hydrological Simulation Program – Fortran (HSPF) (Bicknell et al., 2001) was selected among a range of available models codes since the model has all the requirements needed for application in the study area (which will be expressed in detail in chapter 3), especially with respect to the following aspects:

- Simulation at hourly steps, important to the capture of variant dynamics during flood events
- Consideration of point source and nonpoint sources
- Consideration of all related-processes in nutrient transformation, transport in upland areas as well as in river are considered
- Detailed user manual descriptions
- Free availability from the U.S. EPA

A summary of important processes in upland as well as instream that can be simulated in HSPF is as follows (US EPA, 2009):

- **Nonpoint Loading Simulation**
- Runoff quantity - surface and subsurface
- Sediment erosion/solids loading
- Runoff quality
- Atmospheric deposition
- Inputs needed by instream simulation

Instream Simulation

- Hydraulics
- Sediment transport
- Sediment-contaminant interactions
- Water quality constituents and processes
- Point source accommodation
- Lake/reservoir simulation
- Benthic processes and impacts

However, because the model is very comprehensive, various input data and parameters are required, such as forcing meteorological data, soil information, hydrological, and hydraulic data to sediment, contaminant parameters. In addition, some model algorithms are based on empirical approaches; e.g. soil erosion and transports are modelled based exponential relationships. Details such as implementation or important model algorithms of the HSPF model will be presented in chapter 4 and appendix 4.

2.6.5.4. Model evaluation

Model evaluation is used to assess model performance, i.e. model results are compared to measured data. In general, there are two main approaches in model evaluation. There are statistical methods and graphical analysis. A review on these techniques in water quality modeling can be found in Loague and Green (1991) and recently in Moriasi et al. (2007).

Statistical approach provides a quantitative evaluation. This method relies upon criteria which are calculated based on observed and simulated data. Popular criteria used in catchment water quality modeling are Nash – Sutcliffe efficiency (NSE or Coefficient of efficiency), index of agreement (d), Coefficient of determination (R^2 , the square of the Pearson's product-moment correlation coefficient), Percent bias (PBIAS). These criteria are presented in Table 2.12. Moriasi et al. (2007) recommend using PBIAS for water quality parameters and others can be applied to stream flow comparison. An example of using these criteria in assessment of model performances is provided in Table 2.12. In addition, water quality data contains a high level of uncertainty (e.g. illustrated in Harmel et al., 2006a), and direct comparison may not be appropriate. Furthermore, as mentioned in the section "data collection," water quality data are not often available as complete time-series data. In this case, comparison of frequency distributions these percentiles (e.g., 10th, 25th, 50th, 75th, and 90th) is recommended (Moriasi et al., 2007).

Given certain limitations of statistical methods as pointed out in Loague and Green (1991), there are four methods of graphical display: (1) comparison of observed and predicted concentration profiles; (2) comparison of ranges and medians of integrated values of predicted and observed data; (3) comparison of matched predicted and observed integrated values; and (4) comparison of cumulative distribution functions for integrated values.

Table 2.12: List of criteria used to compare predicted results with observed measurements

ID	Criteria	Equation	Sources
1	Nash Sutcliffe efficiency, NSE (Coefficient of efficiency)	$NSE = 1.0 - \frac{\sum_{i=1}^n (O_i - P_i)^2}{\sum_{i=1}^n (O_i - \bar{O})^2}$	(Nash and Sutcliffe, 1970)
2	Index of agreement, d	$d = 1.0 - \frac{\sum_{i=1}^n (O_i - P_i)^2}{\sum_{i=1}^n (P_i - \bar{O} + O_i - \bar{O})^2}$	(Legates and McCabe, 1999; Willmott, 1984)
3	Coefficient of determination, R^2 (The square of the Pearson's product-moment correlation coefficient)	$R^2 = \left\{ \frac{\sum_{i=1}^n (O_i - P_i)^2}{\left[\sum_{i=1}^n (O_i - \bar{O})^2 \right]^{0.5} \left[\sum_{i=1}^n (P_i - \bar{P})^2 \right]^{0.5}} \right\}^2$	(Legates and McCabe, 1999)
4	Percent bias (PBIAS)	$PBIAS = \frac{\sum_{i=1}^n (O_i - P_i) \times (100)}{\sum_{i=1}^n (O_i)}$	(Gupta et al. 1999, cited in Moriasi et al., 2007)
5	RMSE (Root Mean Square Error) -observation standard deviation ratio (RSR)	$RSR = \frac{\left[\sqrt{\sum_{i=1}^n (O_i - P_i)^2} \right]}{\left[\sqrt{\sum_{i=1}^n (O_i - \bar{O})^2} \right]}$	(Singh et al. 1999, cited in Moriasi et al., 2007)

Where: O_i : Observe, P_i : Predict, \bar{O} : average of the observe value, \bar{P} : average of the predicted value

With reference to Moriasi et al. (2007), the meaning of the criteria is as follows:

NSE: NSE ranges between $-\infty$ and 1.0 (1 inclusive), with $NSE = 1$ as the optimal value. Values between 0.0 and 1.0 are generally viewed as acceptable levels of performance, whereas values <0.0 indicate that the mean observed value is a better predictor than the simulated value, which indicate unacceptable performance.

d: A computed value of 1 indicates a perfect agreement between the measured and predicted values, and 0 indicates no agreement at all.

R²: The correlation coefficient ranges from −1 to 1. A value of 1 implies that the linear equation describing the relationship between *simulated* (*X*) and *observed* (*Y*) values is perfect. A value of −1 implies that all data points lie on a line on which *Y* decreases as *X* increases. A value of 0 implies that there is no linear relationship between the variables.

PBIAS: The optimal value of PBIAS is 0.0, with low-magnitude values indicating accurate model simulation. Positive values indicate model underestimation bias, and negative values indicate model overestimation bias.

RMSE: The lower the RMSE the better the model performance

RSR: RSR varies from the optimal value of 0, which indicates zero RMSE or residual variation and therefore perfect model simulation, to a large positive value. The lower RSR, the lower the RMSE, and the better the model simulation performance.

Table 2.13: General performance ratings for recommended statistics for a monthly time step (Moriassi et al., 2007)

Performance Rating	RSR	NSE	PBIAS (%)		
			Streamflow	Sediment	N, P
Very good	0.00 < RSR < 0.50	0.75 < NSE < 1.00	PBIAS < ±10 ±10 <	PBIAS < ±15 ±15 <	PBIAS < ±25 ±25
Good	0.50 < RSR < 0.60	0.65 < NSE < 0.75	PBIAS < ±15	PBIAS < ±30	< PBIAS < ±40
Satisfactory	0.60 < RSR < 0.70	0.50 < NSE < 0.65	±15 < PBIAS < ±25	±30 < PBIAS < ±55	±40 < PBIAS <
Unsatisfactory	RSR > 0.70	NSE < 0.50	PBIAS > ±25	PBIAS > ±55	±70 PBIAS > ±70

In conclusion, for simulated flow assessment, the NSE is still the most often used criteria. For predicted water quality, PBIAS is adopted. The graphical assessment is recommended for all. Furthermore, uncertainty boundary or probability distribution of observed data should be clearly defined (e.g. illustrated in Harmel and Smith, 2007).

In addition, contaminant loadings for each event can also be calculated (see also in Walling and Webb, 1981; Zhang et al., 2008). The loading (kg/h) for each constituent is calculated as follows:

$$Load = 3.6 \times \sum_{i=1}^n \frac{(Q_{i-1} + Q_i)}{2} \times \frac{(C_{i-1} + C_i)}{2} \quad (\text{eq. 2.76})$$

Where:

- n = Number of stormwater samples
- Q_i = Instantaneous discharge, m³/s
- C_i = Instantaneous concentration, mg/l
- 3.6 = Conversion constant for calculating loads in kg/h

2.7. Deficits in implementing current model approaches in tropical areas

2.7.1. Tropical regions and modeling approaches

The term “tropical region” or “tropic” is defined for those regions lying within 23° north and south of the equator. The subtropical regions are those from 23 to 40° north and south of the equator, the temperate regions lie beyond latitude 40° (Lal, 1990).

Many (not all) tropical regions are characterized by two distinctive seasons, namely rainy and dry season. During rainy seasons, extremely heavy rainfall events and floods often occur. As mentioned in section 1.2 of this chapter, the most important aspects in runoff generation are rainfall (intensity, duration), hydraulic conductivity of soil, land cover and topography. Thus, runoff generation is distinguished in different climate regions. Walsh (1980) observes different behaviours of overland flow on dry and humid tropical regions, while Bonell et al. (1993) mention that the runoff generation in tropical forest are mainly caused by Horton overland flow and saturation overland flow. Dubreuil (1985) based on extensive fieldwork in the intertropical Africa also confirms that the distinctive features of the tropical regions can differ significantly from other regions in term of hydrological behaviours.

The extreme characteristics of climate and hydrological components in tropical regions significantly affect to the processes of nutrient dynamics including soil erosion. Lal (1990) compiles an extensive book on “soil erosion in tropical regions”. He (Lal, 1990) identifies that because the extreme climate and hydrological conditions, soil erosion in the tropics are often very drastic as compare to those in temperate regions. In addition, misuse of soil also contributes to the increasing of soil erosion in the tropics. Rose (1993) compares rainfall, runoff and sediment generation between tropic and temperate regions and concludes that rainfall, runoff and sediment are much higher in the tropic than in temperate regions. Lewis (2008) provides an analysis on physical and chemical features of flow water in the tropics whereas the dynamics of nutrients (e.g. nitrogen, phosphorus and carbon) are highlight.

Walsh (1980) indicates that very different models operate in different parts of the tropics. Although some of these variations can be explained in terms of systematic changes in soil factors with increasing wetness and decreasing seasonality of the climate, other factors, particularly lithology, topography and heavy rainfall magnitude or frequency also play major roles. Walsh (1980) also states that although there are a number of studies on runoff generation mechanism, most of these works have been conducted in humid temperate areas, particularly Great Britain and Eastern United States. In addition, it is observed in this chapter that most flood events are accompanied with sediment and contaminants, especially in agricultural areas. Therefore, applied research methods must be adapt to the tropical condition. For example, Harden (1990) develop an extrapolation method to estimate soil erosion from field scale to catchment scale. Another example as showed in Figure 2.4 in section 2.1. should be kept in mind when applying models in tropical regions.

Researchs on nutrient dynamic modeling at small catchment scale during flood event in tropical regions are limited. Modeling works in tropical regions mostly focus on stream flow and sediment dynamics. For example, Campling et al. (2002) apply TOPMODEL model to simulate rainfall – runoff relationship; Marsik and Waylen (2006) use CASC2D model to assess the changes of land cover on hydrological cycles; Millward and Mersey (1999) use the RULSE model with some modifications to adapt tropical conditions; Diaz-Ramirez et al. (2008b) provide an example of utilization of HSPF model to study hydrology, soil erosion, and sediment transport for tropical island watersheds at

monthly time steps. Polyakov et al. (2007) apply AnnAGNPS model on simulation of runoff and sediment in tropical catchment, however, it is also limited at daily and monthly time steps. Other works on nutrient dynamics are based on analysing sampled data (Kang and Lal, 1981; Maimor, 1996) in a statistical manner or applying model at farm scale, e.g. nitrogen leaching (Mai, 2007). Thus, the development of models to simulate nutrient dynamics at small catchment scale during flood events, especially at hourly time step, in tropical regions is not really considered yet and this aspect is at that core of this thesis.

2.7.2. Data availability, model selection and model development

Data scarcity is a common problem as emphasized in the section “ ungauged catchment.” The lack of data in developing countries is not restricted to any particular area or scales (temporal and spatial) (Kundzewicz, 2007b; Peters et al., 2007). In catchment water quality modeling, data availability decreases according to (1) meteorological data; (2) discharge data; (3) water quality data; in which the meteorological data is the most regularly monitored data. In the pilot catchment, the issue of data scarcity is also found. Therefore, additional data should be collected and further detail will be presented in **chapter 3** of this thesis.

Based on an analysis of literature, the HSPF model is selected among a number of available model codes. However, adapting this comprehensive model to the tropical conditions (i.e. Vietnam) will be a challenge due to, for example, requirements of input data, identification of model parameters. The implementation of this model for the specific area will be presented in **chapter 4**.

Beside data scarcity, site-specific and operational requirements are also considered in an attempt to develop a model. The previous reviews are substantially and significantly helpful in this aspect. Specifically, the understanding of dominant processes, model complexity, modeling issues, etc. will all be taken into account for model development. For this, a new model adapted to the specific demands of tropical regions will be developed, tested and presented in **chapter 5**.

2.7.3. Issues of Catchment water quality management in Vietnam

In Vietnam, conflicts in water resources management have been increasing in the recent years, based on the report done by the World Bank and other institutions (1996) and Pho et al. (2003). Vietnam would seem to have an advantageous surface water situation, given the extensive network of rivers, favourable topography and rainfall patterns in relation to its population size. However, in a recent documentation prepared by the Ministry of Environment and Natural Resources (MONRE), the World Bank and the Danish International Development Assistance (DANIDA) (2003), Vietnam is facing many water issues such as water pollution, floods, and droughts (Nguyen, 2006). A reference is made to the Dong Nai river basin as an example of one of the three main river basin systems in Vietnam that is being plagued with those issues. Pollutants come from various sources such as industrial, domestic waste-water, fertilizer wash-off from agriculture. Most of these sources are uncontrollable resulting in a serious decrease in water in the last few years. In “the Environment Report of Vietnam, the state of water environment in 3 river basins of Cau, Nhue-Day, Dong Nai river system” carried out by the Vietnam Environment Protection Agency (2005) emphasizes Vietnam’s unsustainable water resource. In addition, given extensive agricultural activities in the country, existence of diffuse pollution is quite clear (MONRE, 2003). However, this aspect does not get enough attention even in the most recent years (MONRE, 2009b; VEPA, 2005), in both water quality monitoring program and modeling efforts. Furthermore, although illegal wastewater disposal during flood events is often reported by local residents, no official evidence is available because of limited observations. These problems lead to

inadequate water quality management, e.g. wastewater allocation, or surface water restoration. Therefore, in this thesis, an exploration of the role of catchment water quality modeling for water resources management in Vietnam is made and presented in **chapter 6**.

3. Study area: data collection, and monitoring

3.1. Study area – the Tra Phi catchment, Tay Ninh province, Vietnam

3.1.1. Selection of study area

In this PhD project, several criteria were fixed in order to find a study area. They were:

- Existing of both point and diffuse pollution;
- Contributing to water pollution problems in the area;
- Possibility to set up measurement stations and suitability for logistic preparation.

After a few weeks of surveying in the South Eastern region of Vietnam, consulting from the local experts and officers, the author selected a small catchment.

The study catchment, namely Tra Phi, is a tributary to the Tay Ninh river catchment. The Tay Ninh river catchment, a tributary to Vam Co Dong river, is one of the most polluted spots within the Dong Nai river basin, the 3rd largest national river basin in Vietnam (VEPA, 2005) (see Figure 3.1). Recent observations of the Institute for Environment and Resources (IER) and Tay Ninh DONRE (Department of Natural Resources and Environment) (Huynh et al., 2007) showed that the water quality in downstream part of this catchment is often highly polluted (e.g. dissolved oxygen is less than 2mg/l). However, due to limited fundings, considerations, there are only a few sampling activities carried out in this catchment (e.g. maximum of 2 samples x 2 times/year) just to evaluate what the level of pollution is. In addition, the Tay Ninh river catchment, has been recently selected as a research area in an ongoing joint research project (German Ministry of Education and Research – BMBF and Vietnam Ministry of Science and Technology – MOST) about “Water pollution control management in key economics zones of South Vietnam”. This project is coordinated by the Leichtweiß-Institute for Hydraulic Engineering and Water Resources (LWI), Technical University of Braunschweig and the Institute for Environment and Resources (IER), Vietnam National University of Ho Chi Minh city (Le, 2007). Results from this work will partly contribute to the joint research project as well.

Tra Phi catchment covers about 21 km². The catchment is identified by its corner coordinates of (11°19'58" N, 106°5'30" E), (11°23'30" N, 106°10'15" E). Up to now, there do not exist any research and monitoring program regarding water pollution and management in this catchment. Thus, the catchment is regarded as an **ungauged** catchment.

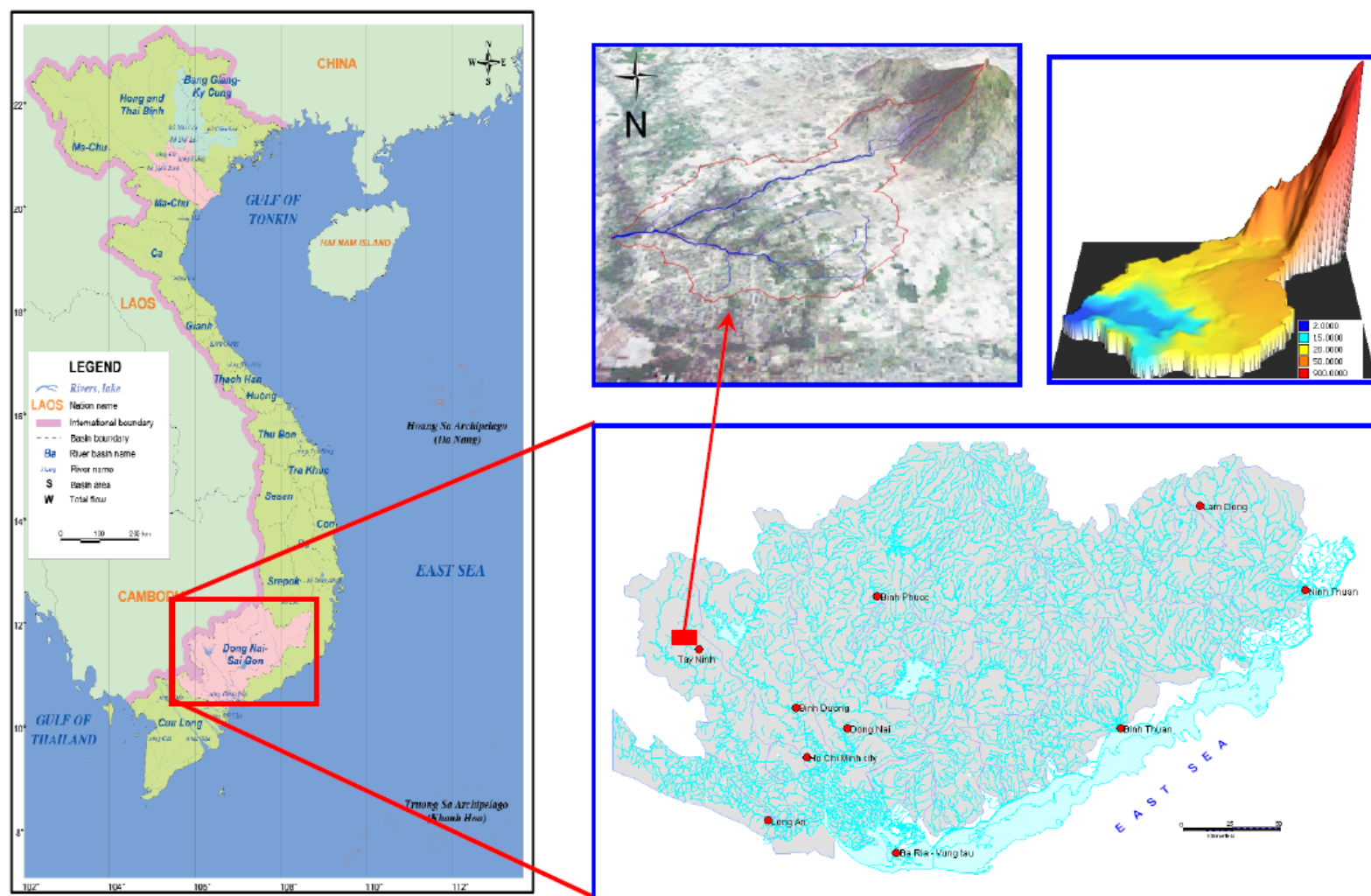


Figure 3.1: Study area (top right) in relation to Tay Ninh water surfaces (top middle), Dong Nai river basin (down right) and Vietnam and main river basins (left) (VEPA, 2005)

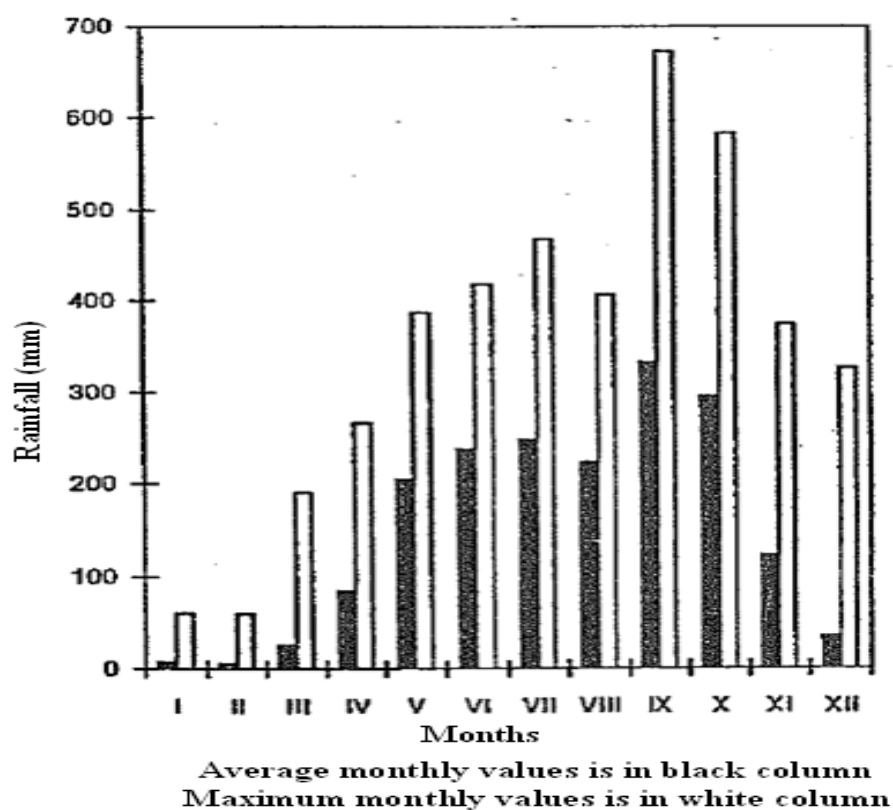


Figure 3.2: Average monthly rainfall at Tay Ninh station (TN DOSTE, 2000, p.51)

3.1.2. Climate

The catchment is affected by the tropical monsoon climate with two distinguish seasons (rainy season from May to November, dry season from December to April). The maximum annual rainfall in Tay Ninh is about 1950 – 2650mm and 90 - 96% percent is within rainy season. Heaviest rainfall occurs in September and October with a total average is about 300 – 400 mm and a maximum of 600 – 700mm (see Figure 3.2). Extreme rainfall events often occur in the area whose maximum daily rainfall observed during 1978-1998 was 180mm (TN DOSTE, 2000).

3.1.3. Topology

The catchment is characterized by highly topographical variation ranging from 2m-30m above sea level (a.s.l) in the low-land areas, to 1000m a.s.l in the water head (Figure 3.3). The extremely high areas belong to the mountainous regions of Nui Ba Den this region takes only small parts of the catchment.

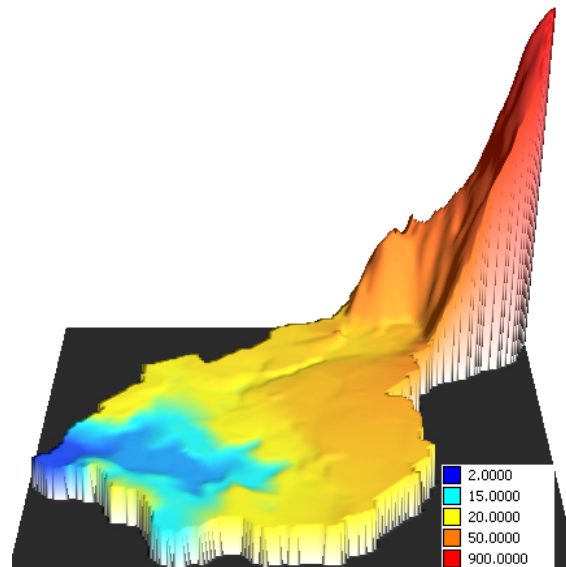


Figure 3.3: Topography variations of Tra Phi

3.1.4. Drainage characteristics

The Tra Phi catchment is a 3rd order catchment. Drainage density is about 1250 m/km². There is a drainage irrigation canal system through the catchment transferring water from Dau Tieng reservoir for irrigation purposes (Figure 3.4; Figure 3.5). This system is independent from the river network in term of direct contribution to river flows. In this study, it is assumed that the contribution of irrigated water to river network is neglected.

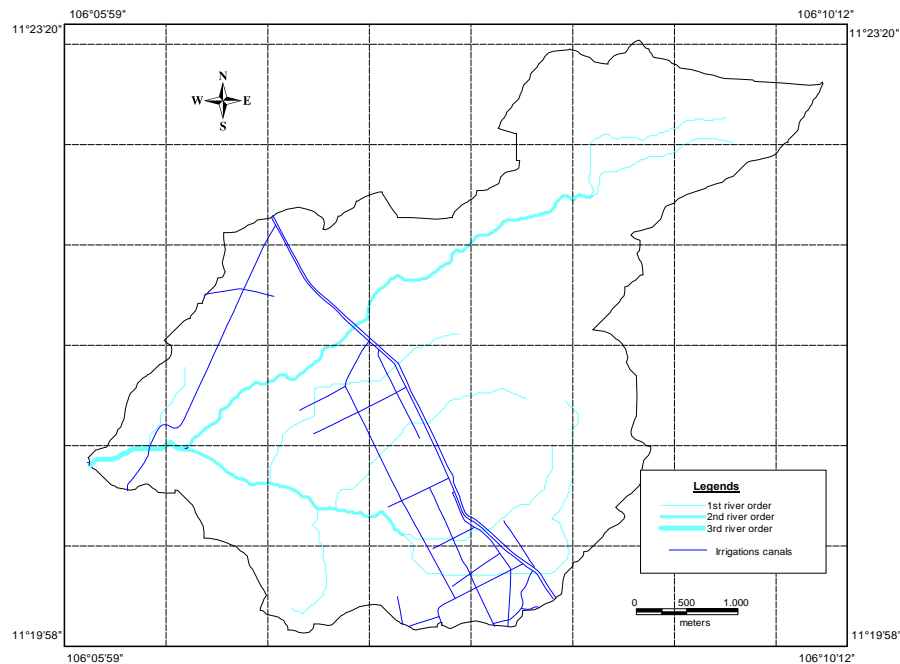


Figure 3.4: The Tra Phi river system (extracted from digital elevation model) and existing irrigation canals

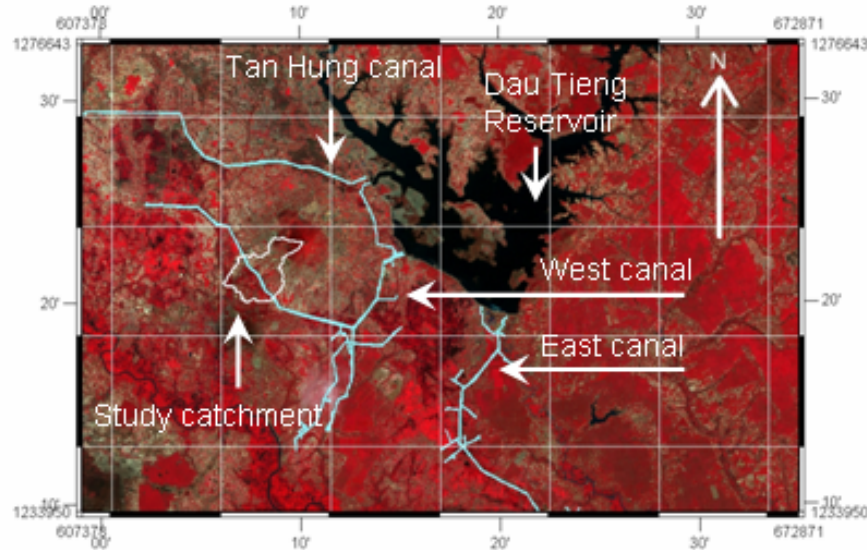


Figure 3.5: The study area in relation with Dau Tieng reservoir and Tan Hung, West, East canals

3.1.5. Land use, land cover

There are three main land-use units including agriculture (66 %), forest areas (11%), semi-urban areas¹⁰ (13%). Detailed distributions are illustrated in Figure 3.6 and Figure 3.7 and are described as follows:

- Rice (20%), sugar apple, sugar cane, rubber, cassavas are the main agricultural plants in this catchment.
- “Tree” includes short term plants such as sugar cane, cassavas (15%);
- “High trees” are mainly rubber (31%);
- “Water” is river and existing canals, ponds (3%);
- “Rock” is open rock mines in the low areas of the mountain (1%);
- “Semi-urban” area covers separated houses (13%).

Most of the areas are pervious; the impervious areas are mainly the houses themselves since surroundings of the houses are agricultural lands.

¹⁰ Semi-urban area is defined here as mainly pervious areas except main roads, houses

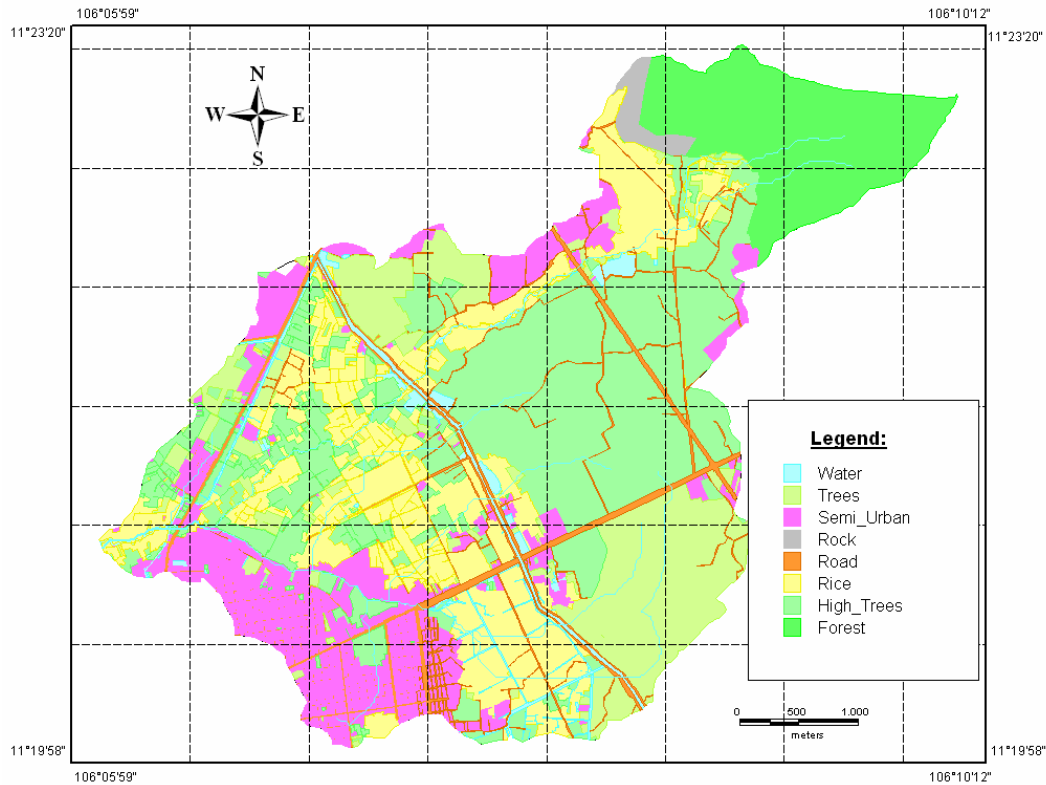


Figure 3.6: Land cover units of Tra Phi catchment (Source: Tayninh department of Natural resources and Environment)

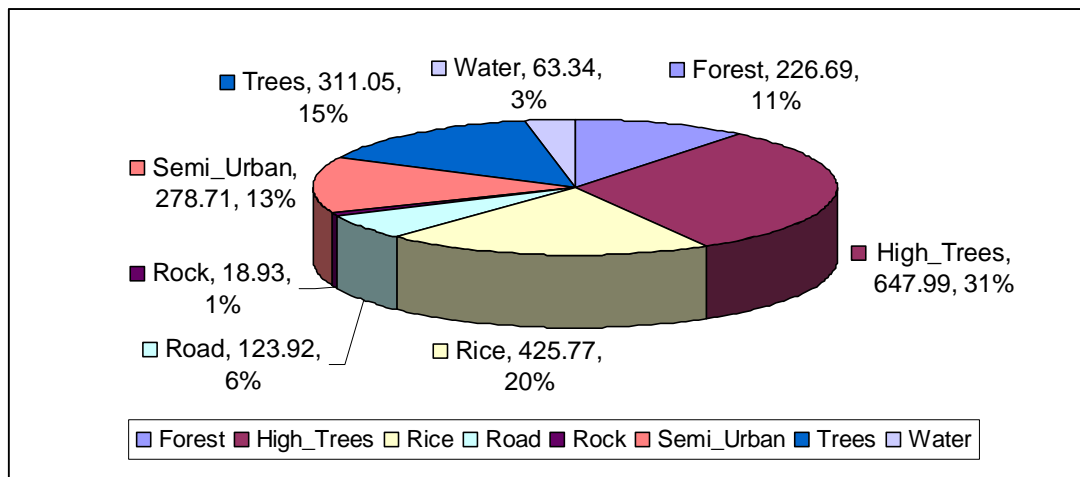


Figure 3.7: Land cover distributions in Tra Phi catchment (in ha and %) (Source: Tayninh department of Natural resources and Environment)

3.1.6. Geology, soil

The main geological units of the Tra Phi catchment are illustrated in Figure 3.8 and are described as follows:

- aQ_{IV}^{2-3} : Early Holocene age, with a narrow, uncontinuous, limited areas. This is the alluvial sediment, of which the silt-clay is dominant: silt-clay $40 \div 60\%$, silt: $20 \div 30\%$. Upper part: sandy-clay, silt-clay, alluvial sediment, 1.4m depth.
- $aQ_{II-III}^{1_{td}}$: Middle and late Pleistocene, this is the Thu Duc strata. The main component is clay mixed with sand. Detailed contribution from top to down: sand increases from $2,9 \div 37,3\%$, silt decreases from $39,9 \div 26 \%$, clay decreases from $71,1 \div 22.8 \%$.
- Alluvial sediment: pebble, sand, clay, laterite.
- Q_1 : Early alluvial sediment, upper part: pebble, sand, clay, 10-30 meter depth.
- $\gamma\delta J_3 dq$: Dinh Quan complexes, Granodiorit biotite, Hornblend-Pyrocen – this is rocky mountain (Nui Ba Den).

The alluvial sediment from aQ_{IV}^{2-3} , $aQ_{II-III}^{1_{td}}$, Q_1 is the basic for creating the current soil in Tra Phi catchment. According to *TN DOSTE* (2000), these formations, after the mechanical and other weathering processes (in the humid, monsoon tropical regions), created in Tay Ninh mostly grey soil (acrisols). This aspect is reported also elsewhere (FAO, 2000; Macías, 2008; Phan, 1992). Therefore, in this thesis, the characteristics of acrisols are applied. For example, the surface soil texture is mainly sandy loam.

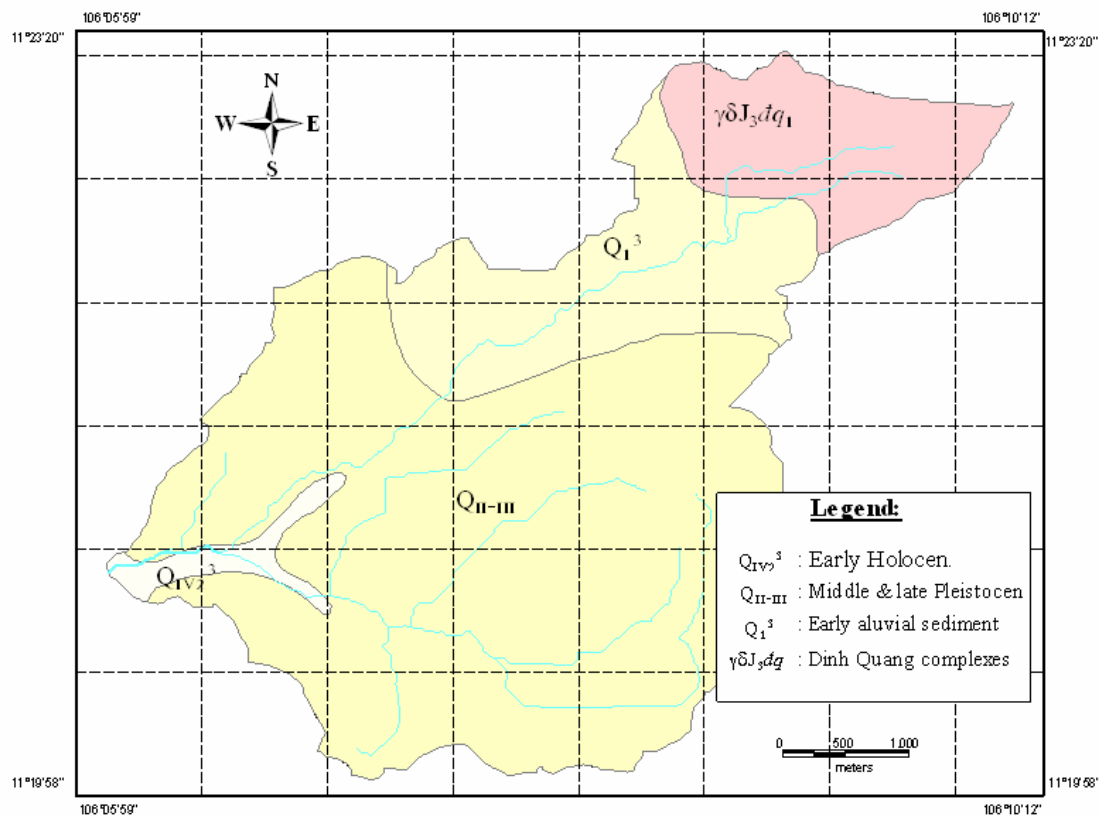


Figure 3.8: Geological map of Tra Phi catchment (Huynh et al., 2007)

An acrisols soil profile in Vietnam is shown in Figure A2.23 and its description is presented in Table A2.1 and Table A2.2 in appendix 2.

3.1.7. Point sources

The only one identified point source comes from a tapioca production factory (Figure 3.9). The company produces averagely 30 tons tapioca starch per day which generates about 360-600 m³ wastewater (Huynh, 2006). Normally, from April to July each year, the company often stops working due to limited supply of raw tapioca. In 2008 (the year of fieldwork campaign), the company was operating from middle of July, however, but stopped working in August due to low-demand market. Most of the wastewater from the company is kept inside linked ponds (Figure 3.9) for sometime. Parts of it evaporate and other part infiltrate into the soil. If the ponds are filled up a large amount of the wastewater is directly diverted into the river system. In daily operating, a part of wastewater (estimated about 3 m³/hour)¹¹ from a washing tapioca-bulb pond is directly and continuously discharged into the river since the pond is always full during operating period. Concentrations of several parameters of 2 samples collected in 2007 and 2008 are shown in Table 3.1. It was observed from the field that the wastewater can be easily increased during heavy rainfall. Unfortunately, there was no measurement taken during the event.

Table 3.1: Wastewater data of 2 samples collected by the author

Parameters	Samples	
	(1)	(2)
Temperature	30.8	27.6
pH	4.12	4.8
Dissolved oxygen, mg/l	1.2	3.03
Total suspended solid (TSS) , mg/l	2260	3675
Total dissolved solid (TDS) , mg/l	269	185
Total phosphorus , mg/l	5.35	14.6
Phosphorus - Phosphate P-PO ₄ , mg/l	11.3	11.8
Total Nitrogen Kjeldahl N-Kj, mg/l	67	58.3
Nitrate NO ₃ ⁻ , mg/l	1.02	0.34
Ammonium NH ₄ ⁺ , mg/l	18.8	22.9

(1) 17:30 11.09.2007; (2) 6:15 27.07.2008 (local time, UTC+7)

¹¹ The 3 m³/hour was estimated by only one random observation. Regular monitoring was not possible due to private sector (see figure A2.20 to figure A2.22 appendix 2)



Figure 3.9: Location of the tapioca starch company, its linked ponds (blue areas), river Tra Phi network and measuring station (overlying on satellite image – Source: Google maps)

3.2. Data collection and monitoring

The monitoring campaign including installation of the measuring station, samplings and analysis of water samples was completely performed by the author. It is emphasized that the monitoring program had to be adapted to the limited financial funds for experimental work within this study. So, the data collection and data availability of this work is representative for the existing conditions of research work in developing countries.

3.2.1. Data collection

3.2.1.1. Archived data

Available data in the catchment are:

- Meteorological data at the Tay Ninh National meteorological station located 2 km away from the catchment outlet. Data from the station include: (1) daily evaporation; (2) hourly rainfall; (3) hours of sunshine; (3) wind direction and speed 4 times/day; (5) hourly temperature; (7) hourly humidity (see Figure A2.23, appendix 2).
- Land use map from the Tay Ninh Department of Natural Resources and Management at 1:10.000 scale
- Topographic map from the Vietnam National Information and Communication Technology Department at 1:25.0000 scale that is basically used for generating a Digital Elevation Model (DEM)
- Remotely sensed data: Landsat TM images in 2002 from internet (<http://www.landsat.org/ortho/index.php>) and Google Map

3.2.1.2. Field survey

Field survey crossing the catchment during the field campaign is for:

- Investigating land covers in the areas: Main crops, land covers in comparison with satellite images using handheld GPS (see from Figure A2.1 to Figure A2.10, appendix 2).
- Investigating stream: canal networks, rills/interills generation which cannot be seen in topographic maps were observed during events
- Interviewing farmer : cropping season (lunar calendar), applied fertilizers varying among each others (deviation for the same crops is about 1 week)
- Sampling water/soil upstream: in order to roughly evaluate water and soil quality upstream. (sample data are presented in appendix 3)

Figure 3.10 shows locations where water sample and soil samples were taken during the campaign.

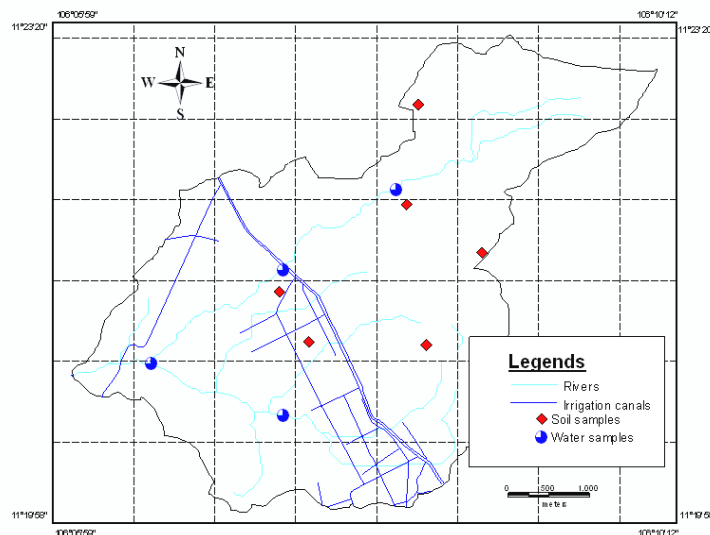


Figure 3.10: Locations of water and soil samples

3.2.2. Monitoring

The monitoring activities were mainly done at the outlet of the catchment as shown in Figure 3.9, Figure 3.10 and from A2.15 to A2.18, appendix 2. A few water samples collected upstream are presented in previous section (Figure 3.10), thus they are omitted here. The activities at outlet station include discharge measurement, water sampling and analysis.

3.2.2.1. Discharge measurement

Flow discharge of the Tra Phi catchment was measured at the catchment outlet only using an Acoustic Doppler Current Profiler (ADCP) which could be made available from ongoing BMBF – MOST joint research project (Meon and Le, 2010). A temporary station was built for measurement during 2007 and 2008 rainy season (Figure A2.16, appendix 2). The ADCP operates across the channel during low and normal flow (e.g. velocity less than 0.6 m/s); flow measurement was taken in the middle of the channel during high flow. Based on 25 gaugings (ranging from 1 to 4.5 m³/s), a stage – discharge curve was developed (Figure 3.11). According to Herschy (1978), the Standard Error of Mean

Relation (SE_{mr}) was 7% that means the developed curve can be used with $\sim 93\%$ of confidence. In addition, according to Harmel et al. (2006a) the velocity – area method used for discharge calculation under high flow condition may provide an error of up to about 10%. Therefore, cumulative errors for discharge data may have a magnitude of about 16%.

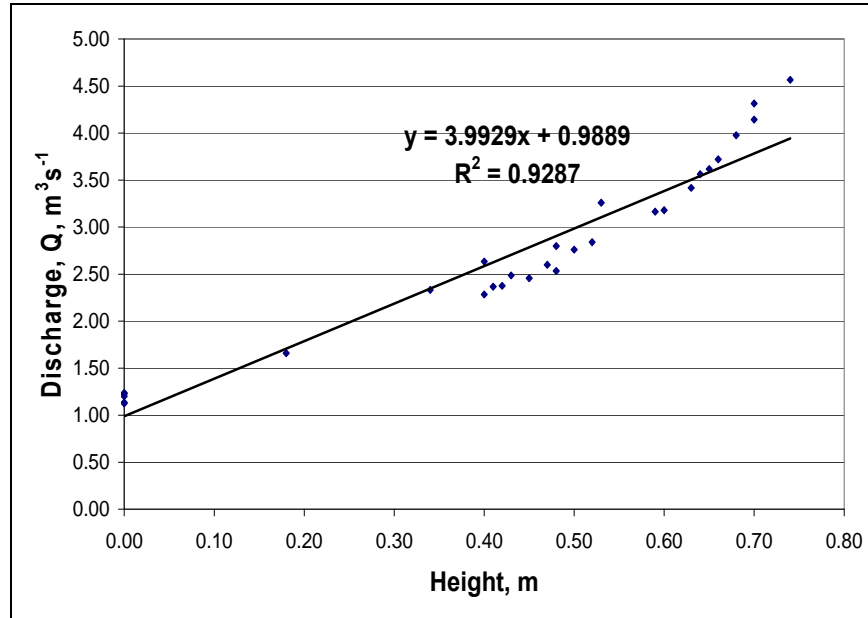


Figure 3.11: Stage – discharge curve

3.2.2.2. Event descriptions

The following three events were comprehensively measured:

- Event 1: 18:00, 25 July 2008 – 7:00 27, July 2008 (local time, UTC+7);
- Event 2: 17:00, 6 August 2008 – 6:00 9, August 2008 (local time, UTC+7);
- Event 3: 10:30, 14 August 2008 – 9:00, 15 August 08 (local time, UTC+7)

Synthesized information on these three events is presented in Table 3.2

Table 3.2: Summarized information of three observed events

	Event 1	Event 2	Event 3
Total rainfall, mm	58.6	18.6	33.6
Stream water level variation, cm	68	9	80
Hourly maximum rainfall intensity, mm	40.5	7.3	27.6

It should be noted the rainfall data used is only based on one station. It was observed that rainfall distribution was not equally distributed in the catchment during the events. This “quantitative” observation is also confirmed by checking radar rainfall images and daily rainfall station. The differences varied among the events. In addition, according to TN DOSTE (2000), rainfall data errors at measurement station can be up to 7%. Therefore, these errors should not be neglected. Figure 3.12 shows the rainfall variation taken by radar images in the region during the event 25 July 2008.

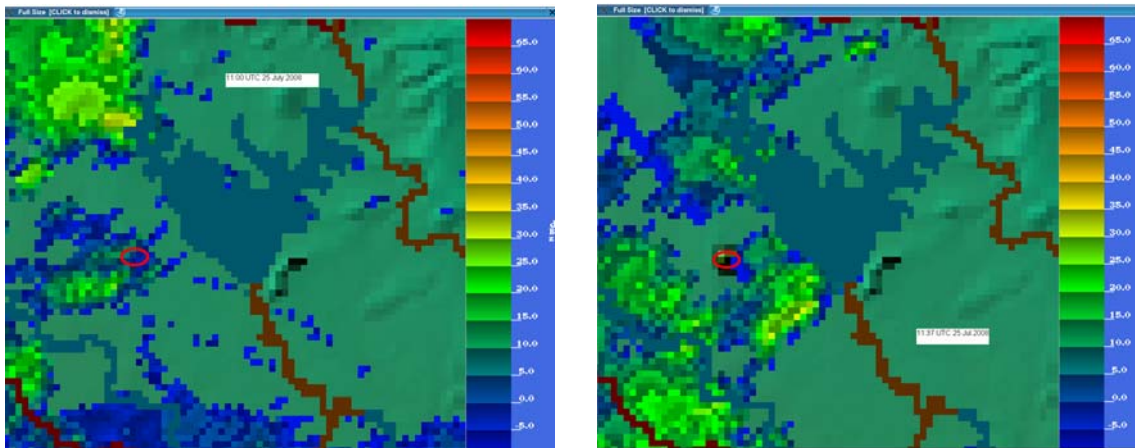


Figure 3.12: Rainfall distribution in the region during the first event on 25 July 2008 (the red circle is the study catchment) (11:00 UTC, 25th July 2008 on the left and 11:37 UTC, 25th July 2008 on the right)

3.2.2.3. Sample collection

Water sampling was done based on observation of flow discharge as well as at a certain time interval. Sampling frequency during 3 events is presented in Figures 3.13 to 3.15. Water samples were collected variably before, during and after flood events every 1, 2, 3 hours depending on water level changes (e.g. 1 or 2 hour interval when water level rises rapidly; 3, 4 hour interval when water level recedes slowly). Shih et al. (1994, cited in Arvo, 2005) concluded that “for a good estimation of load **at least eight time-integrated samples** are needed per runoff event to reach the level of accuracy comparable to a single flow-composite sample and consequently we can lose any advantage over grab sampling at such high sampling frequency”. Thus, the water sampling frequency in this study is acceptable.

Only one sample was taken for each time in the middle of the stream, at a depth of 40 cm from water surface (see figure A2.18, appendix 2). In the first event, water samples were not well collected in the rising curve with regard to the discharge variation. The reason is due to the rapid rise of flow.

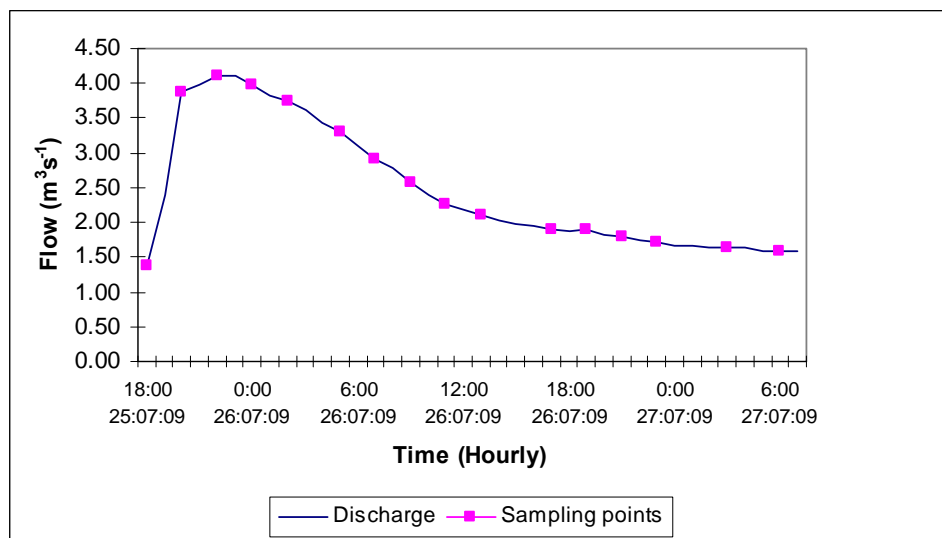


Figure 3.13: Flow discharge in relation to sampling points event 1 (16 samples)

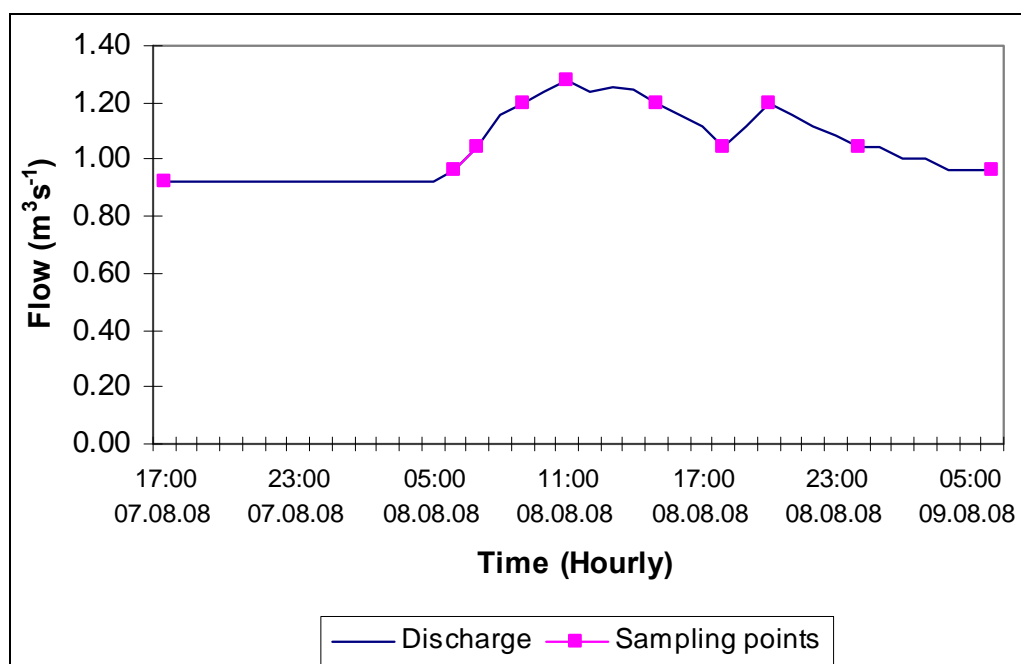


Figure 3.14: Flow discharge in relation to sampling points event 2 (10 samples)

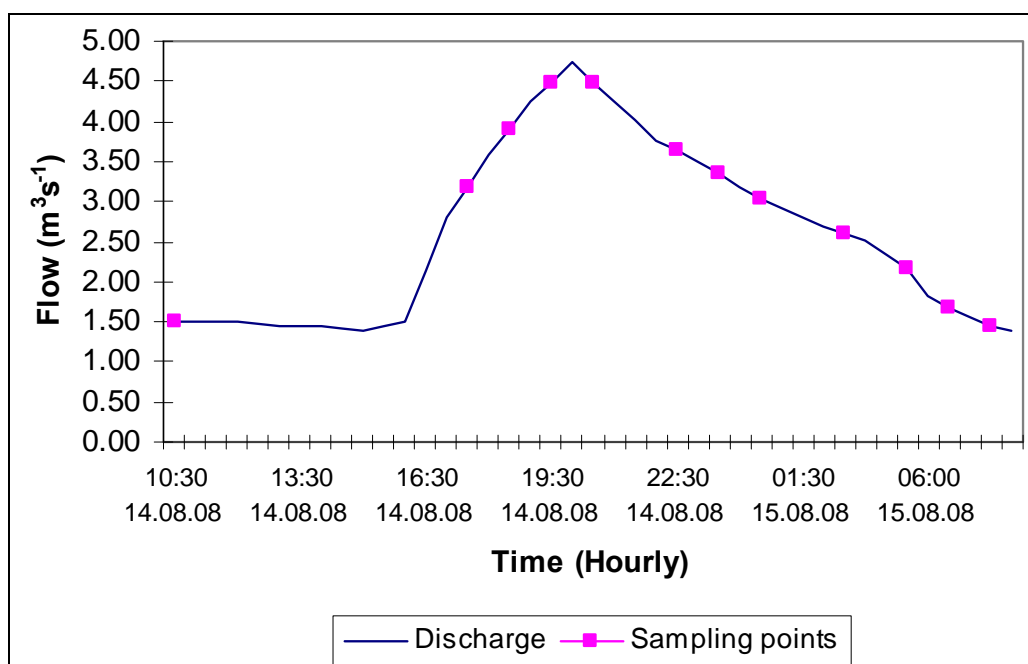


Figure 3.15: Flow discharge in relation to sampling points event 3 (12 samples)

3.2.2.4. Water quality measurement and analysis

Several parameters were analysed immediately after sampling: temperature (T^0), pH, dissolved oxygen (DO), total dissolved solid (TDS) using a handheld instrument (WTW 197). P-PO₄, N-NH₄, N-NO₃ were analysed within 24 hours using a photometer (Spectroquant NOVA 60) (see figure A2.19, appendix 2). Total suspended solid (TSS), total phosphorus (TP), total nitrogen (TN) were analysed within 5-10 days at laboratory of the Institute for Environment and Resources (IER) in Ho Chi Minh city following the Standard Methods (2005).

According to methods presented in Harmel et al. (2006a), cumulative measured data errors are due to sampling, preservation and analysis and presented in Table 3.3. Here, the error of phosphorus phosphate is the highest (50%), followed by the total suspended solid (28%), nitrogen ammonium (18%) and finally nitrogen nitrate (18%). These errors will be shown as error bar when evaluating model results in chapter 4 and 5.

Table 3.3: Cumulative errors of measured data for selected parameters

	TSS (%)	P-PO ₄ (%)	N-NH ₄ (%)	N-NO ₃ (%)
Sampling	15	15	5	5
Preserve	5	30	10	10
Analysis	8	8	8	7
Cumulative errors	28.09	50.39	18.41	18.00

3.2.2.5. Summary

Rainfall and flow discharge data are presented in Figure 3.16 to Figure 3.19, while TSS, P-PO₄, N-NH₄, N-NO₃ are shown in Figure 3.20 to Figure 3.22. Based on these observations, the following remarks are given:

Three different magnitudes of rainfall and consequently flow for each event were observed. The maximum rainfall ranged from 7 mm, 40 mm to 26 mm, while discharge varied from 1.3 m³/s, 4.1 m³/s to 4.7 m³/s, respectively. The correlation coefficient between the maximum rainfall intensity and maximum river discharge is very high ($R^2 \sim 0.96$). Time lag (or time to peak), the differences in time between maximum rainfall and maximum discharge, is about 2 – 4 hours and depends on event durations. One should note that there were also other events which occurred in between these events. However, only rainfall data are available as shown in Figure 3.16. This aspect will be taken into account, especially when considering the runoff generation e.g. based on SCS curve number method.

Behaviours of total suspended solid (TSS), phosphorus phosphate (P-PO₄), nitrogen ammonium (N-NH₄) and nitrogen nitrate (N-NO₃) were highly dynamic during these events. TSS was the most sensitive parameter to event durations and as well as event magnitudes. However, P-PO₄, N-NH₄, N-NO₃ behaved at certain differences. During the first and third events, the concentrations of P-PO₄ and N-NH₄ varied in corresponding to flow discharge (i.e. 0.4 - 1 mg mg/l and 0.1- 1.4 mg/l for P-PO₄, N-NH₄ respectively). In contrast, during the second event, these variables increased in a much higher magnitude (i.e. 0.25 - 3.6 mg/l and 0.1 - 2.3 mg/l for P-PO₄, N-NH₄ respectively), although this was the smallest event. The concentration of N-NO₃ reached the highest value of 2.4 mg/l during the first event.

During the second event, a strong smell of tapioca starch was noted in the sampled water. Based on this, it can be assumed that the different behaviours between the second on one hand and the first and third events on the other hand were highly influenced by more wastewater disposal.

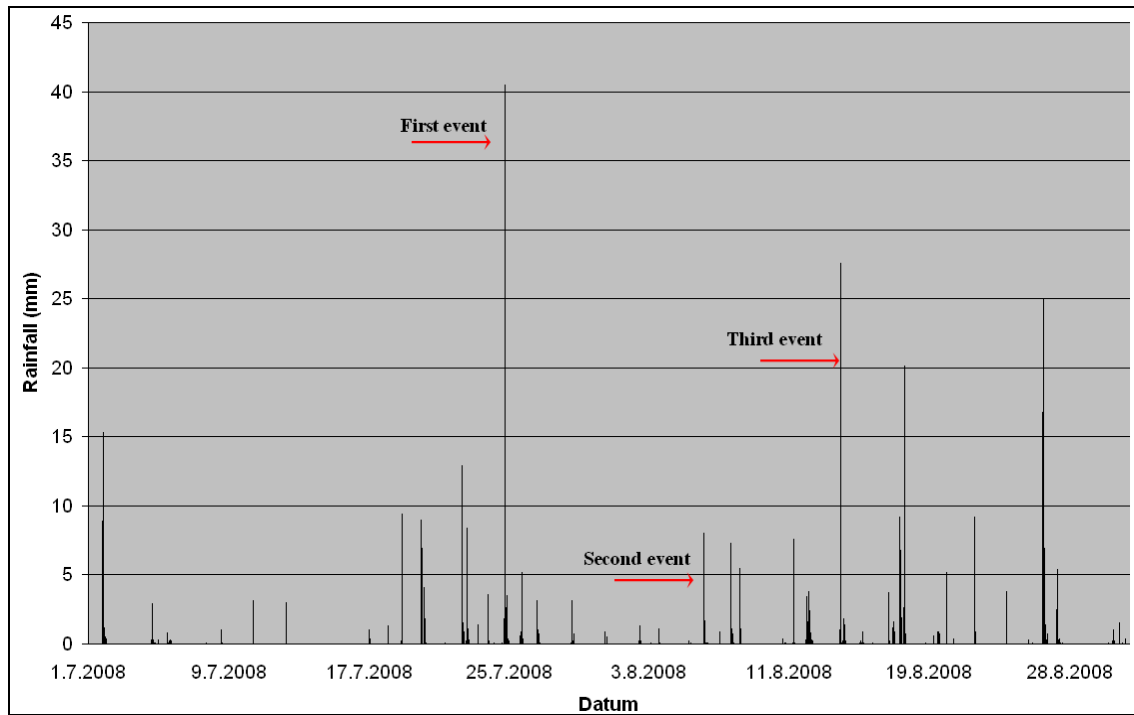


Figure 3.16: Hourly rainfall at Tay Ninh station from 01.07.2008 – 31.08.2008, and three observed events

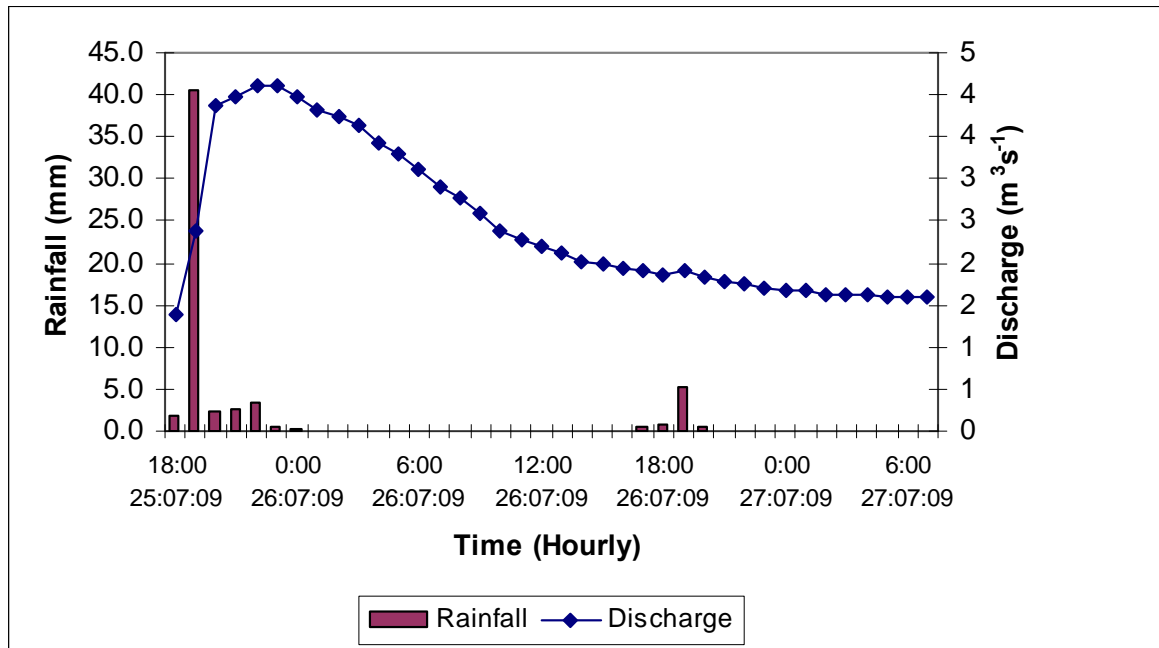


Figure 3.17: Rainfall and flow discharge measured at catchment outlet (25/7/2008 – 27/7/2008)

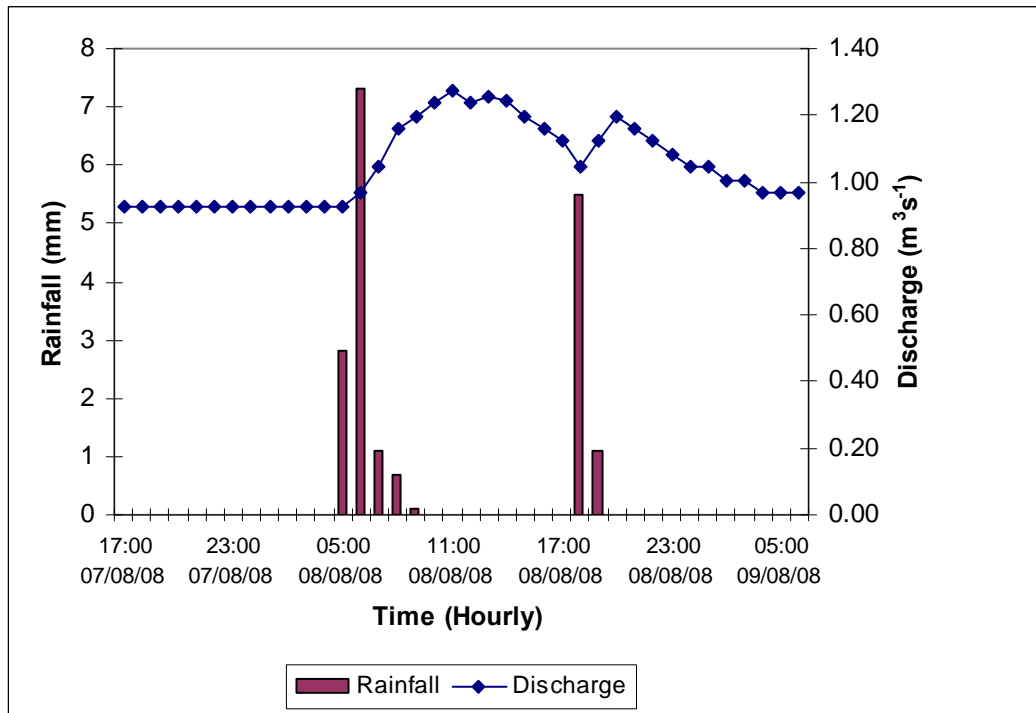


Figure 3.18: Rainfall and flow discharge measured at catchment outlet (7/8/2008 – 9/8/2008)

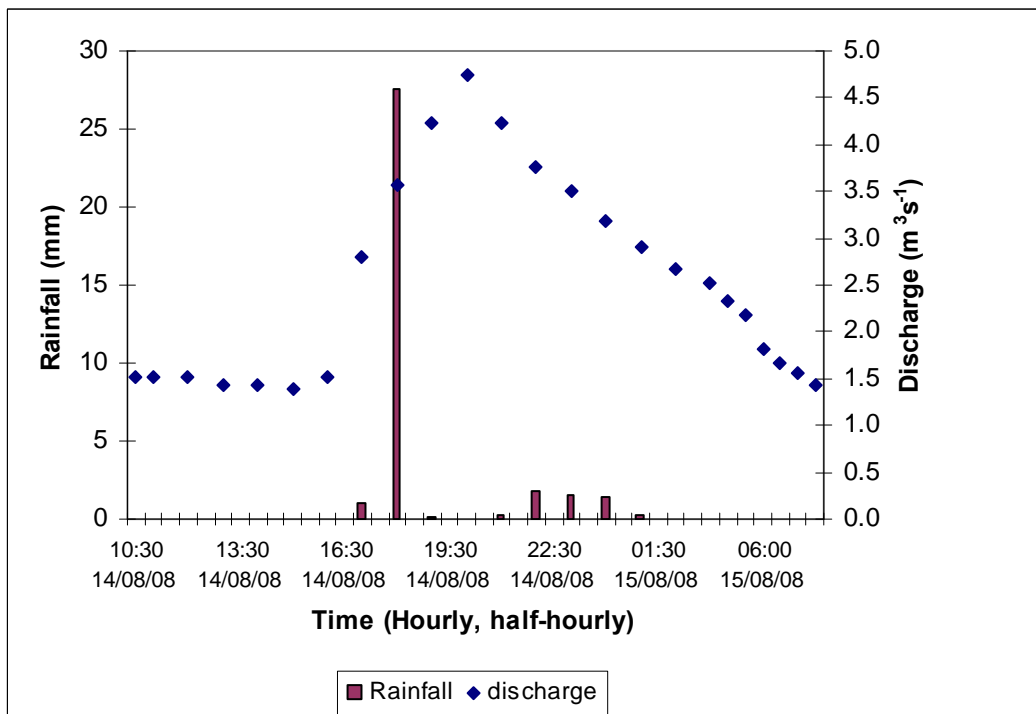


Figure 3.19: Rainfall and flow discharge measured at catchment outlet (14/8/2008 – 15/8/2008)

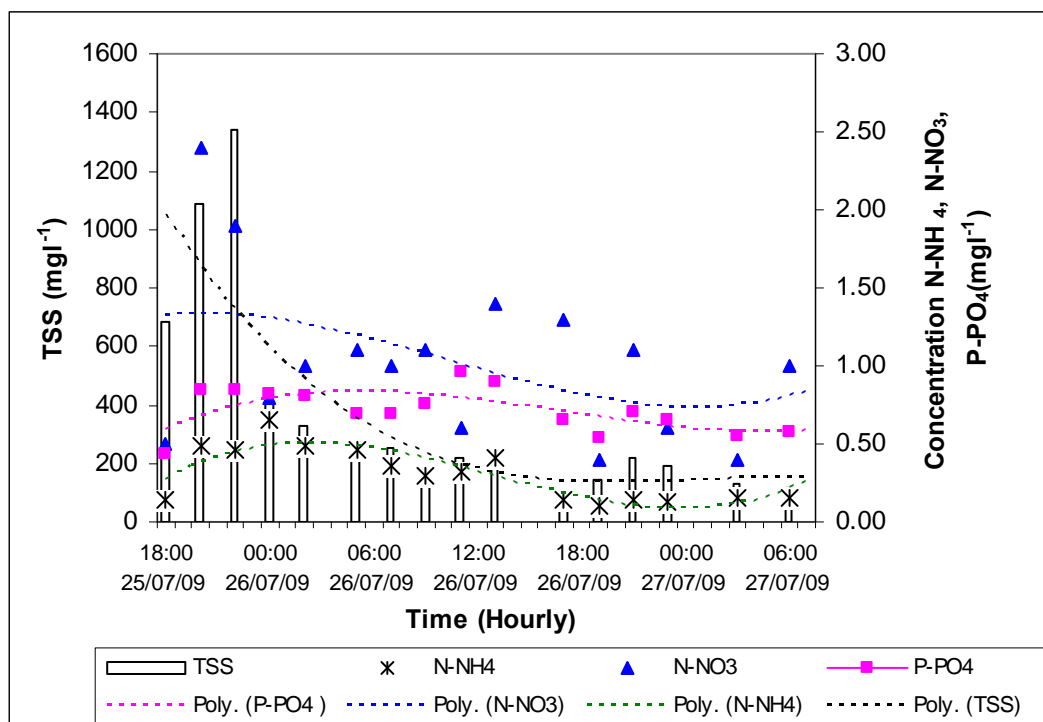


Figure 3.20: TSS, N-NO₃, N-NH₄, P-PO₄ measured at catchment outlet (25/7/2008 – 27/7/2008) and polynomial function fitted to measured data

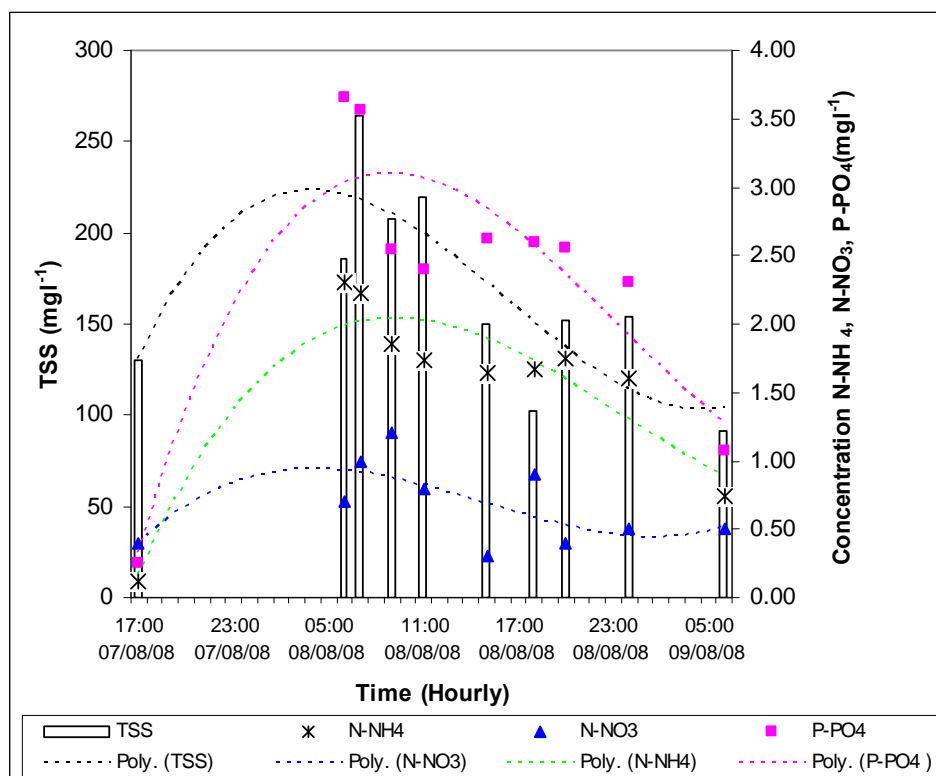


Figure 3.21: TSS, N-NO₃, N-NH₄, P-PO₄ measured at catchment outlet (7/8/2008 – 9/8/2008) and polynomial function fitted to measured data

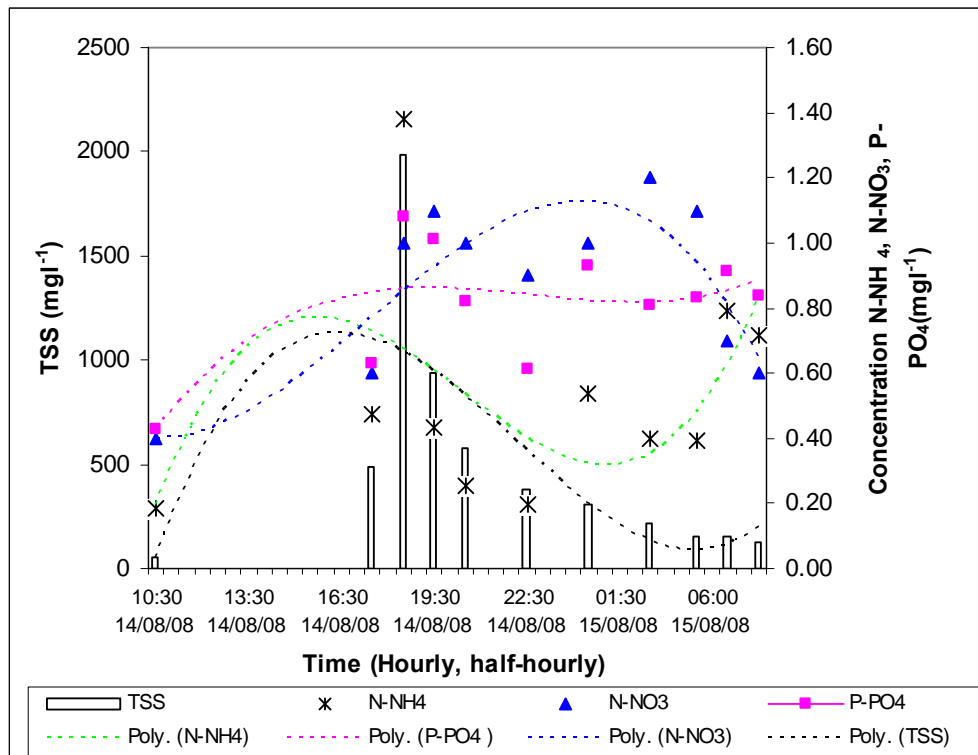


Figure 3.22: TSS, N-NO₃, N-NH₄, P-PO₄ measured at catchment outlet (14/8/2008 – 15/8/2008) and polynomial function fitted to measured data

Table 3.4, Table 3.5 summaries the monitoring data as shown from Figures 3.20 to 3.22, where the trends of monitoring data were fitted using polynomial functions. The derived correlation coefficients are based on exponential fitting curve between constituents and flow as well as between constituents and TSS, and those are presented as $R^2(Q)$, $R^2(TSS)$, respectively.

Table 3.4: Summary of measured data during 3 events (TSS and P-PO₄)

	TSS			P-PO ₄			
	min	max	$R^2(Q)$	min	Max	$R^2(TSS)$	$R^2(Q)$
	(mg/l)	(mg/l)		(mg/l)	(mg/l)		
Event 1	86	1340	0.41	0.43	0.96	0.10	0.48
Event 2	91	264	0.19	0.25	3.65	0.38	0.12
Event 3	58	1988	0.78	0.43	1.08	0.47	0.12

Table 3.5: Summary of measured data during 3 events (N-NH₄ and N-NO₃)

	N-NH ₄				N-NO ₃			
	min	max	$R^2(TSS)$	$R^2(Q)$	min	Max	$R^2(TSS)$	$R^2(Q)$
	(mg/l)	(mg/l)			(mg/l)	(mg/l)		
Event 1	0.11	0.65	0.30	0.81	0.40	2.40	0.29	0.33
Event 2	0.13	2.30	0.41	0.19	0.30	1.20	0.24	0.03
Event 3	0.18	1.38	0.21	0.01	0.40	1.20	0.26	0.38

The findings are summarized as follows:

- **TSS:** Between TSS and discharge (Q), the highest R^2 was 0.78 for event 3 and R^2 was 0.41, 0.19 for event 1, 2, respectively. It should be noted that as described in section 3.1.7 “point sources”, event 3 was not affected by point sources disposal. Therefore, the sediment was in very high correlation with the river discharge.
- **P-PO₄:** The highest correlation between P-PO₄ and Q was obtained in event 1 ($R^2= 0.48$) and the coefficient remained low in event 2, 3; while the highest correlation between P-PO₄ and TSS was 0.47 (event 3) and the coefficient was 0.38 and 0.1 for event 2, 1 respectively. Thus, the explanation for P-PO₄ using TSS and flow discharge is very difficult.
- The correlation between **N-NH₄** and Q, as well as between N-NH₄ and TSS was different with those observed P- PO₄. While with flow discharge, the R^2 was 0.81, 0.19, 0.11 (event 1, 2, 3, respectively), with TSS was 0.41, 0.3, 0.21 (event 2, 1, 3, respectively)
- There was no significantly clear relation between **N-NO₃** and Q as well as between N-NO₃ and TSS. The correlation coefficient R^2 with flow discharge was 0.33, 0.3, 0.38 (event 1, 2, 3, respectively) and with TSS was 0.29, 0.24, 0.26 for event 1, 2, 3, respectively.

In addition, another similar test was given to the observed nutrient parameters. Results are shown in Table 3.6 leading to the following remarks:

- Among the 3 nutrients, P-PO₄ and N-NH₄ are most correlated, especially during the second event (R^2 was 0.98) where the contribution of point sources was expected. This correlation was also observed in the wastewater sample (Table 3.1)
- Correlation between N-NO₃ and P-PO₄ as well as between N-NO₃ and N-NH₄ was not clear: with P-PO₄, R^2 was 0.29, 0.24, 0.26 (event 1, 2, 3, respectively); with N-NH₄, R^2 was 0.33, 0.3, 0.38 (event 1, 2, 3, respectively)

Table 3.6: Correlation coefficient among P-PO₄, N-NH₄ and N-NO₃

	P-PO₄ & N-NH₄	P-PO₄ & N-NO₃	N-NO₃ & N-NH₄
Event 1	0.49	0.27	0.23
Event 2	0.98	0.2	0.25
Event 3	0.48	0.38	0

The data indicate a poor correlation between flow, suspended sediment and nutrient constituents (i.e. smaller than 0.5). However, the suspended solid (sediment) is considerably correlated with flow discharge when no/little point source effects. The correlation coefficient can explain up to 40 ~ 80%.

A relation between nutrient constituents and discharge or sediment is hardly visible. However, it was observed the correlation between P-PO₄ & N-NH₄ is quite high as compared to N-NO₃, especially for the second event where there was also a good agreement between these two parameters in the wastewater samples.

Although data availability for statistical analysis is quite limited (only 3 events), it must be accepted that monitoring alone is not enough to explain the variation of water quality owing to system complexity and various anthropogenic impacts. Therefore, **other tools (i.e. modelings) are needed to investigate the nutrient dynamics.**

4. Application of the Hydrological Simulation Program – Fortran (HSPF) model

4.1. Model description

The Hydrological Simulation Program – Fortran (HSPF) was selected among a range of available models codes as presented in section 2.6.5.3, chapter 2 since the model responses to all requirements needed to the objectives of this study. Bicknell et al., (2001) stated that “the HSPF is the primary catchment model included in the EPA BASINS modeling system. HSPF is a comprehensive catchment model of hydrology and water quality, simulating land surface and subsurface hydrologic and water quality processes, linked and closely integrated with corresponding stream and reservoir processes. BASINS/HSPF is a major tool for catchment and TMDL assessments across the US”. For example, the HSPF model has been used in a number of applications, especially in (1) Hydrology simulation; (2) Nutrient transport; (3) Best Management Practice at catchment/river basin scale (AQUA TERRA, 2005; Diaz-Ramirez, 2007; Donigian et al., 1995). Since HSPF is a continuous model, it is used mostly for long-term water balance and nutrient transport studies. In this thesis, its ability in event simulation is investigated using a time step of one hour.

The Hydrological Simulation Program – Fortran (HSPF) (Bicknell et al., 2001) is a continuous or event-based model for simulating catchment hydrology and water quality for nutrients, toxics, bacteria, sediment. The model can perform at hourly or daily time steps for each sub-catchment and river reaches which can be easily discretized using the BASINS modeling system (as presented in section 2.6.2.2). Regarding nutrient contaminants, the model takes into account all processes relating to nutrient dynamics at catchment scale comprising of hydrology, erosion and sedimentation, nutrient variations in soil and water (including in river flowing water). Furthermore, model spaces are discretized based on land use characteristics, the model can also perform scenario analysis, e.g. Best Management Practice.

Since one of objectives of this thesis is to simulate nutrient dynamics during flood events using the HSPF model, the focus of the following section is given to describe important processes and modules implemented in the HSPF model responding to this objective. Figure 4.1 provides a sketch about water flow and nutrient transport performed in the HSPF model. There are four important modules shown in Figure 4.1 including model input, water budgets, nutrients and model outputs. Model input are meteorological (e.g. precipitation, evaporation, radiation, wind speed) and nutrient data (i.e. accompanying with land-use types, point sources). Model input data for this application is presented in section 4.2 of this chapter. Water budgets are basically a representation of the hydrological cycle at catchment scale as presented in chapter 2. This module is described in more detail in appendix 4, which includes also description of the spatial resolution and about the processes. The nutrient module includes nutrient associated with water and sediment and also nutrient reactions (transformations) in soil and water. The following section will focus about the setting – up of model and its application to the Tra Phi catchment

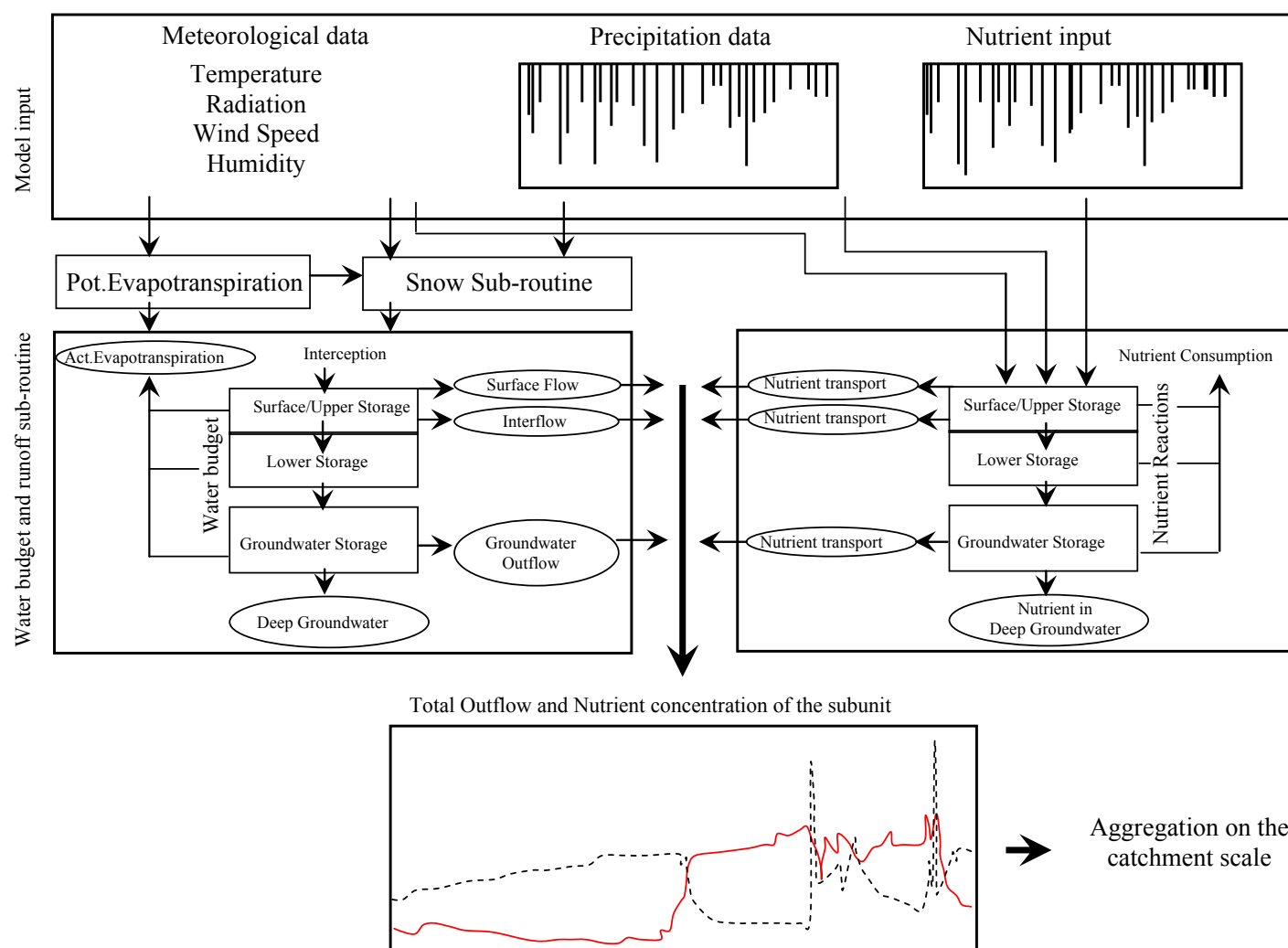


Figure 4.1: Model concept of runoff simulation and nutrient transport in NPSM/HSPF (Eisele et al., 2001) (NPSM: Nonpoint Sources Model)

4.2. Model setup (development)

4.2.1.1. Data requirement

HSPF requires three main categories of data as input: landscape data (topography, point source locations, streams, etc.), meteorological data (precipitation, air temperature, humidity, etc.), and landuse and pollutant specific data (landuse areas, monitoring data, etc.)

Various data sources for model development were collected. Those are:

- Meteorological data which were obtained from Tay Ninh meteorological national station which is 1 km away from the outlet;
- Landuse and topographic maps obtained from local agencies
- Soil parameters adopted from user manual (Bicknell et al., 2001) and through calibration
- Point sources loadings being estimated based on the sampling campaign (chapter 3)

However, since soil data is not available for a long term simulation (e.g. soil temperature), nutrient transformation processes in soil are not considered. Thus, the model only uses the “PQUAL” module based on relatively simple process algorithms. Other modules in the PERLND (section 4.1.1.1) like MSTLAY, PEST, NITR, PHOS and “TRACER” are not utilized.

4.2.1.2. Data preparation

HSPF requires two primary input files for simulation: the User Control Input (UCI) file and the Catchment Data Management (WDM) file. The UCI file is used to set up operation process for the model and to assign model input parameters. The initial UCI file is prepared in the BASINS system. In addition, it can be modified in Win-HSPF during model calibration processes. The WDM file prepares input time-series data e.g. rainfall, evaporation, temperature in order to simulate hydrological processes as well as nutrient dynamics. The WDM file also stores output time-series results. The WDM file is processed in the WDMUtil packet (Hummel et al., 2001) which is accompanied with the BASINS system as available from US EPA website (US EPA, 2007).

a. Data preparation in BASINS system

The BASINS system operates as an independent Geographic Information System (GIS), namely MapWindow (<http://www.mapwindow.org>), where spatial data such as Digital Elevation Model (DEM), land use maps are processed. Firstly, the DEM is processed in order to identify and extract physical properties of the catchment such as discretizing sub-catchments, drainage network, slope, length etc. The extracted map is then overlaid with the land use map. The pervious and impervious parts within a sub-catchment are defined by the user. Point source data can be imported in this system or in Win-HSPF. Ready data are exported to Win-HSPF as the basis for model simulation. Figure 4.2 shows final land use data and sub-catchments readily exported to Win-HSPF

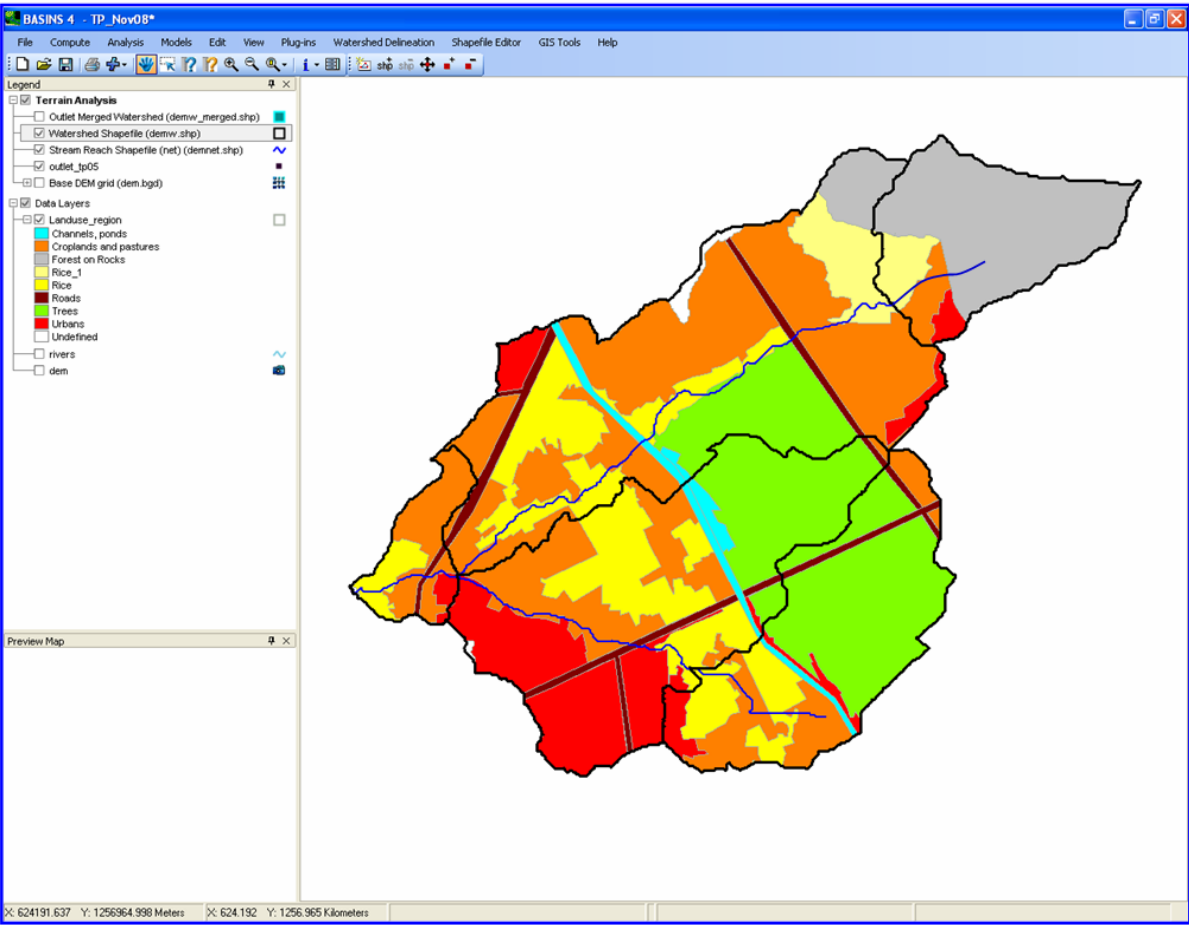


Figure 4.2: Land use map and sub-catchments prepared in BASIN system

b. Forcing (meteorological) data preparation in WDMUtil

WDMUtil is software accompanying with the BASINS system. The package can handle multiple time-series data within a “*.wdm” file. The WDM file contains data used for model simulation i.e. forcing data and stores simulation output. Figure 4.3 shows which data are required for which applications. Output data can be generated for any component in the simulation process that is defined in the user’s manual (e.g. fluxes/storages at sub-catchment outlet or reaches).

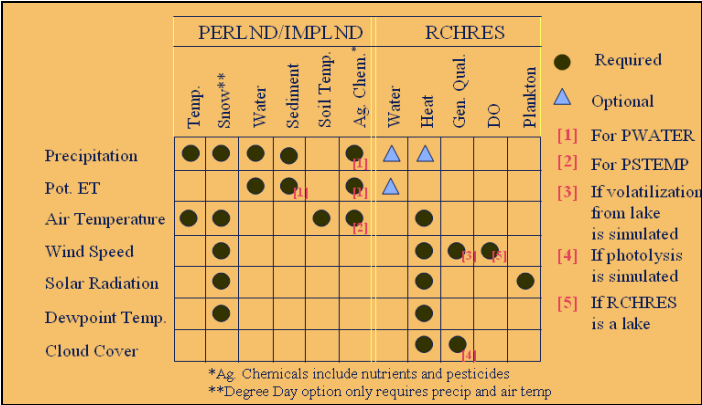


Figure 4.3: HSPF weather data requirements (US EPA, 2009)

In this thesis, hourly meteorological data which are available in Excel format are imported to WDMUtil using some modified scripts (Hummel et al., 2001): rainfall, air temperature, humidity, wind speed. Hourly potential evapotranspiration and evaporation are calculated as follows: the potential evapotranspiration is calculated using the Hamon method provided within the WDMUtil, while the evaporation is computed by disaggregating 12 hours-measured data. These two data is later compared to make sure that the evaporation does not exceed the potential evapotranspiration. The calculated summary of available data is presented in Table 4.1

In order to simulate nutrient dynamics in soil profiles, other time series data is needed e.g. soil temperature. Such soil time-series data is not available, thus the simple nutrient transformation and transport in HSPF is implemented, for example, only the PQUAL module is used for simulating nutrient dynamics in upland areas.

Table 4.1: Meteorological data and frequency for HSPF

Type of data	Location of data collection	Units	Frequency
Precipitation (rainfall)	Tay Ninh	mm	hourly
Temperature	Tay Ninh	oC	hourly
Dewpoint temperature	Tay Ninh	oC	hourly
Wind speed	Tay Ninh	m/s	hourly
Humidity	Tay Ninh	percentage	hourly
Cloud cover	Tay Ninh	percentage	hourly
Potential evapotranspiration	calculated	mm	hourly
Evaporation	calculated	mm	hourly

4.2.2. Model discretization

The Tra Phi catchment is discretized in the BASIN system into five sub-catchments accompanied with five reaches as shown in Figure 4.4. Physical information of the catchment and land use distribution are summarized in Table 4.2.

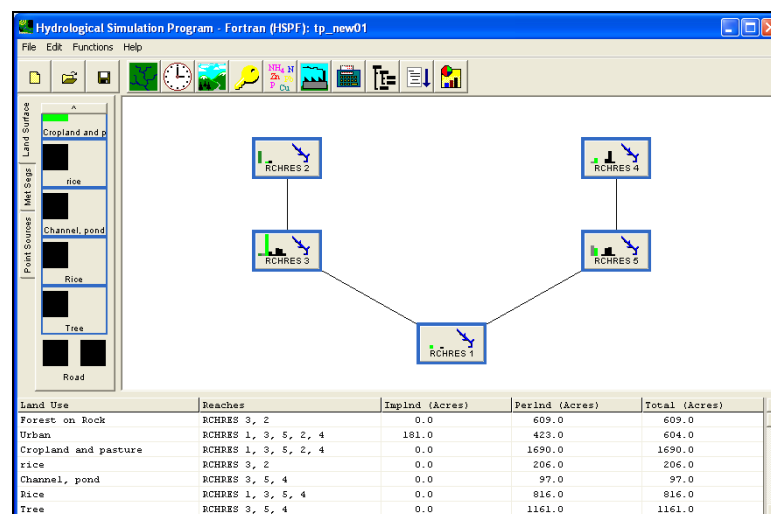


Figure 4.4: The conceptual modeling units for Tra Phi catchment in Win- HSPF

Table 4.2: Physical characteristics of sub-catchments and reaches

Parameter	Sub-catchment				
	SWS1 (reach 2)	SWS2 (reach 3)	SWS3 (reach 4)	SWS4 (reach 5)	SWS5 (reach 1)
Sub-catchment area (ha)	266	811	389	621	87.9
Drop in water elevation from the upstream to the downstream (m)	19.5	3	1.5	0.8	1.5
Channel length (km)	1.74	5.54	1.54	2.64	1.11
Average channel slope (%)	0.21	0.005	0.006	0.006	0.002

Landuse distribution in relation to sub-basins is described in Table 4.3, where different land use types are summarized within a sub-catchment (horizontal direction) and in the whole catchment (the sum of final row), and percentage of each sub-catchment (the sum of final column). It can be seen that the land use areas for agricultural activities (cropland, rice, trees) cover about 70% of the catchment, while sub-catchment 1,2 covered mostly with rocks take about 10% of total areas. The cropland, pasture and rice are dominant in sub-catchment 1, 3 (more than 70%), while forest on rock is dominant in sub-catchment 2 (78%), most impervious areas (urban, road) locate in sub-catchment 5 (33%).

Table 4.3: Grouping sub-catchment according to land use types (unit: ha)

Sub-catchment	Forest on Rock	Urban and road	Cropland and pasture	Rice	Channel, pond	Tree	Sum
SWS1 (reach 2)	-	10.93 (13 %)	55.44 (63%)	21.45 (21%)	-	-	87.82 (4%)
SWS2 (reach 3)	209.22 (78 %)	9.71 (4%)	20.64 (8%)	25.9 (10%)	-	-	265.47 (12%)
SWS3 (reach 4)	37.23 (5%)	61.51 (8%)	398.62 (49%)	184.54 (22%)	15.38 (2%)	113.31 (14%)	810.59 (37%)
SWS4 (reach 5)	-	35.61 (9%)	82.15 (21%)	56.66 (15%)	6.07 (2%)	208.01 (53 %)	388.55 (32%)
SWS5 (reach 1)	-	201.96 (33%)	127.07 (20%)	125.05 (20%)	17.81 (3%)	148.52 (24%)	620.39 (29%)
Sum	246.45 (11%)	319.7 (15%)	683.92 (31%)	413.59 (19%)	39.25 (2%)	469.84 (22%)	2172.77 (100%)

4.2.3. Model parameterization

4.2.3.1. Model calibration strategy

In this thesis, model calibration follows the hierarchy of catchment model calibration (US EPA, 2009). Firstly, the hydrological component is calibrated. Next, the simulated sediment loadings are compared to observation ones. Finally, nutrients variables like P-PO₄, N-NO₃, and N-NH₄ are considered. Detailed in-stream model parameters (e.g. chemical, sediment interactions, and transports in stream) were not taken into account since data are available only at the catchment outlet. However, some rough information on some cross sections, water quality measured during field survey periods in upper stream are used as initial conditions.

Sensitive parameters were recommended in BASIN's lecture notes (US EPA, 2009) as well as from Radcliffe and Lin (2007). Model parameters were manually calibrated given values adopted from technical notes (US EPA, 2000a; US EPA, 2000b). The following notes are adapted for model calibration:

- Assign an average value for each parameter with different land use types until “optimal” parameter reached i.e. good agreement between observed and simulated data. Since HSPF is a complex model, by doing this way we would have a rough variation of model parameters so that time will be reduced.
- Modify model parameter values manually according to different land use. However, with soil parameters which are not strongly affected by land cover, the calibrated data are kept (except in the rocky areas) since it is assumed that the Acrisols is dominant in the catchment.
- Base flow and point sources are adjusted based on field experience and monitoring data in order to capture system behaviour before flood events. This is considered as providing initial conditions for the model
- In-stream parameters are ignored (using default value) except providing initial conditions.
- Model results are assessed using graphical (qualitative) and statistical (quantitative) tests (presented in section 4.3)

4.2.3.2. Model parameterization

The following sections will provide model parameters used after (manual) calibration for different model components, including (1) Hydrology and hydraulic parameters, (2) (Suspended) sediment, (3) Nutrients (ammonium, nitrate and phosphate). The key parameters recommended by US EPA (2009) are as follows:

- Surface Runoff + Interflow (Hydrograph Shape): UZSN; INTFW; IRC; LSUR, NSUR, SLSUR
- Groundwater (Baseflow): INFILT, AGWRC
- Sediment Equilibrium/Balance: KRER, KSER
- Constituents simulated by PQUAL/IQUAL: ACQOP, SQOLIM, WSQOP

The most important aspect in hydraulic parameterization is assigning parameter values for FTABLE. This table requires information for every river reach. Based on field investigation, especially detailed measurement at the catchment outlet (reach 1), hydraulic parameters at five reaches are provided in Table 4.4.

Table 4.4: Estimated Ftable information at 5 cross sections based on field observation

	Reach 1	Reach 2	Reach 3	Reach 4	Reach 5
Mean width, m	22.97	9.84	13.12	13.12	13.12
Mean depth, m	3.28	1.31	6.56	6.56	6.56
N channel	0.07	0.07	0.07	0.07	0.07
N Floodplain	0.40	0.40	0.4	0.4	0.4
Bankfull depth, m	9.84	3.28	8.20	8.20	8.20
Maximum floodplain depth, m	16.40	16.40	16.40	16.40	16.40
Left side floodplain width, m	1640.42	1640.42	1640.42	1640.42	1640.42
Right side floodplain width, m	1640.42	1640.42	1640.42	1640.42	1640.42
Channel side slope	0.47	0.47	1.50	0.33	0.33
Floodplain side slope	0.10	0.10	0.1	0.1	0.1

a. Hydrological parameters

The most representative parameters for the hydrological components including LZSN, INTFW, INFILT, AGWRC, UZSN, IRC, LZETP, LSUR, SLSUR, and NSUR are explained and parameterized (calibrated) in Table 4.5. Given detailed instructions (i.e. US EPA, 2000a) model parameterization of the hydrological processes is straight forward. Some parameters (LZSN, UZSN, LSUR, and SLSUR) are calculated using available formula or GIS processing, while other parameters are calibrated based on look-up table or using default values.

Table 4.5: Process and physical parameters used after calibration of the HSPF model for hydrology

Process parameter	Description (units)	Parametric values					
		Forest	Urban and road	Cropland & pasture	Rice	Trees	Wetland
LZSN	Lower zone nominal storage (mm)	381	482	482	482	482	482
INTFW	Interflow inflow parameter	1.5	1.5	1.5	1.5	1.5	1.5
INFILT	Index to soil infiltration capacity (mm/h)	2.44	1.22	12.69	1.71	6.34	0.24
AGWRC	Groundwater recession coefficient (1/day)	0.99	0.99	0.99	0.99	0.99	0.99
UZSN	Upper zone nominal storage (mm)	4.5	7.7	7.7	7.7	7.7	7.7
IRC	Interflow recession parameter	0.3	0.3	0.5	0.5	0.5	0.5
LZETP	Lower zone ET parameter	0.6	0.3	0.6	0.8	0.7	0.9
LSUR	Length of overland flow plane (m)	45	50	45	37	55	15
SLSUR	Slope of overland flow plane	0.41	0.02	0.02	0.02	0.02	0.02
NSUR	Manning's n for the overland flow	0.15	0.1	0.25	0.4	0.3	0.08

The initial value LZSN is calculated based on a formula given by Linsley et al. (1986, cited in Al-Abed and Whiteley, 2002) as:

$$LZSN = \begin{cases} 100 + 0.25P & (\text{Seasonal precipitation}) \\ 100 + 0.125P & (\text{Precipitation distributed throughout the year}) \end{cases} \quad (\text{eq. 4.1})$$

Where:

P = the mean annual precipitation, mm

UZSN is equal to LZSN multiplied by 0.06 at steep slope areas (i.e. forest on rock) and multiplied with 0.08 at moderate slope areas. The geometry parameters (LSUR and SLSUR) are calculated by means of GIS processing and kept without calibration. The values of the calibrated LZSN, INTFW, UZSN, LSUR, SLSUR, and NSUR parameters stay within the ranges. The infiltration parameter (INFILT) is calibrated according to the instructions (US EPA, 2000a) where the soil is most likely within group A and B. Thus, the INFILT was rather high after calibration. This is suitable with the soil characteristics (Acrisols) as well as given observation in field (except the wetland and rice due to clay deposition on the land surface). The AGWRC, IRC was calibrated after using default values in (US EPA, 2000a) until the recession curve can capture the base flow.

b. Sediment parameters

Initial values for these parameters were chosen from US EPA (2000b; 2009). Calibration is done based on the first event observation and these parameters were then kept for the followed events. Since the catchment is covered by the unique acrisols soil, the sediment generation parameters are kept similar

for each land use type except those affected by land covers. The gully erosion, deposition form atmosphere as well as in stream sediment transport processes are ignored here (No evidence of gully erosion was identified during fieldwork campaign). Thus default values are applied for model parameters of these processes and not listed.

Similarly to the hydrological part, most of the sediment parameters are within the ranges provided in look-up table or default values (US EPA, 2000b). However, the KSER (Coefficient in the detached sediment washoff equation) is out of the range (0.01 – 0.5) as it was observed also in (Diaz-Ramirez et al., 2008a). The calibration is straight forward and soon gets to the “optimal” conditions. Calibrated parameters for erosion, sediment processes are presented in Table 4.6.

Table 4.6: Sediment yield parameters used after calibration of the HSPF model

Process parameter	Description (units)	Parametric values					
		Forest	Urban and road	Cropland and pasture	Rice	Trees	Wetland
KRER	Coefficient in the soil detachment equation	0.3	0.3	0.25	0.2	0.25	0.2
JRER	Exponent in the soil detachment equation (<i>default values</i>)	2	2	2	2	2	2
COVER	The fraction of land surface which is shielded from erosion by rainfall	0.8	0.9	0.7	0.5	0.6	0.2
AFFIX	Fraction by which detached sediment storage decreases each day as a result of soil compaction	0.05	0.05	0.05	0.05	0.05	0.05
NVSI	Rate at which sediment enters detached storage from the atmosphere	0	0	0	0	0	0
KSER	Coefficient in the detached sediment washoff equation (Diaz-Ramirez et al., 2008a)	10	10	10	10	10	10
JSER	Exponent in the detached sediment washoff equation (<i>default values</i>)	2	2	2	2	2	2

b. Nutrient parameters

The calibration of hydrological and sediment parameters follows standard procedures as given by US EPA (2000a; 2000b). This is not the case for nutrient parameters as also described by Radcliffe and Lin (2007). In addition, given the site-specific problems such as simulation at hourly time steps, limited data do not allow to simulate nutrient transformations in soil or using default values for in-stream process parameters. Since the focus of this simulation is nutrient dynamics during flood event only, an assumption of the interactions and transformation processes in soil and river is made. Moreover, it is also observed during model calibration (e.g. the changes of in-stream parameters affect model results to a minor extent only).

In order to cope with the problem of nutrient transformation during normal condition (e.g. continuous simulation during dry days) as well as management practice such as fertilizing the soil, the monthly nutrient accumulation rate and nutrient storage (MON-SQOLIM and MON-ACCUM respectively) in the model has been utilized. Model parameters comprising of SQO, POTFW, POTFS, ACQOP, SQOLIM, WSQOP, MON-ACCUM, MON-SQOLIM mostly relate to storage and transport processes. In addition, because of lacking data for identifying contributions from different land uses, each of the model parameters is kept unchanged. An example of model parameters for phosphate are explained and parameterized in Table 4.7. more information on data and parameter is given in appendix 4.

Table 4.7: Nutrient parameters (P-PO4) used after calibration of the HSPF model

Process parameter	Description	Parametric values					
		Forest	Urban and road	Cropland and pasture	Rice	Trees	Wetland
SQO	Initial storage of QUALOF on the surface of the PLS (kg/ha)	0.45	0.45	0.45	0.45	0.45	0.45
POTFW	Washoff potency factor for a QUALSD (kg/ton)	0.03	0.37	0.07	0.2	0.13	0.2
POTFS	Scour potency factor for a QUALSD (kg/ton)	0.02	0.17	0.03	0.09	0.06	0.09
ACQOP	Rate of accumulation of QUALOF (kg/ha.day)	0.045	0.002	0.054	0.045	0.045	0.045
SQOLIM	SQOLIM is the maximum storage of QUALOF, (kg/ha) (<i>recommended value</i>)	0.027	0.027	0.027	0.027	0.027	0.027
WSQOP	Rate of surface runoff which will remove 90 percent of stored QUALOF per hour (<i>recommended value</i>)	0.5	0.5	0.5	0.5	0.5	0.5
MON-ACCUM	Monthly values of accumulation rate of QUALOF at start of each month (kg/ha.day)	0.05	0.05	0.05	0.05	0.05	0.05
MON-SQOLIM	Monthly values limiting storage of QUALOF at start of each month (from July to September) (kg/ha)	0.45	0.45	0.45	0.45	0.45	0.45

Some parameters are only roughly described by US EPA (2009) e.g. POTFW, ACQOP, SQOLIM, WSQOP. Other model parameters are calibrated by trial and error. The later ones are site-specific. Some other studies using HSPF do not provide similar parameter sets for comparison. For example, the work given by Radcliffe and Lin (2007) implementing HSPF for simulating phosphorus dynamics at catchment scale provided only parameters related to nutrient transformation in soil. Therefore, comparative studies i.e. applying the HSPF model in other areas in the regions or an up-scaling of the model are strongly recommended.

4.3. Model results

Model results are compared with measured data for 3 events: (1) Event 1: 25/7/2008 – 27/7/2008; (2) Event 2: 7/8/2008 – 9/8/2008; (3) Event 3: 14/8/2008 – 15/8/2008. The model results are assessed by both qualitative and quantitative means. Qualitatively, model results versus observed variables are presented from Figure 4.5 to Figure 4.16. The figures include continuous simulation graphs as well as separated events. Quantitatively, as recommended in chapter 2, section 2.6.5.4, a number of criteria indices were calculated. A summary of evaluation parameters is shown in Table 4.8. The observed values in the third events are not the same to the model in term of recorded time (measured and predicted values are shifted a thirty minutes). Therefore, in the evaluation table, the contaminants like TSS, nutrients are only applied for the first and second events, evaluation for event 3 are limited to graphical aspect.

Table 4.8: Model evaluation parameters based on criteria given in Table 2.1

	PBIAS	d	R ₂ (1:1)	RMSE	NSE	RSR	Max diff. (%)	Min diff. (%)
Flow								
Event 1	-34.52	0.90	0.64	0.84	0.48	0.72	-20.39	-37.93
Event 2	-12.05	0.61	-0.12	0.29	-1.70	1.642	-30.65	-5.19
Event 3	50.71	0.76	-1.00	0.78	0.18	0.908	28.96	30.10
TSS								
Event 1	6.62	0.83	0.02	223.78	0.52	0.69	33.28	-74.42
Event 2	-217.50	0.23	0.30	254.01	-85.30	9.29	-324.24	-65.93
P-PO₄								
Event 1	-29.66	0.64	0.17	0.38	-2.95	1.99	-64.58	8.00
Event 2	-2.00	0.77	0.86	0.45	0.24	0.87	5.21	-46.73
N-NH₄								
Event 1	-120.88	0.57	-1.47	0.41	-3.82	2.20	-61.04	-256.45
Event 2	-5.49	0.84	0.91	0.26	0.48	0.72	3.13	-41.90
N-NO₃								
Event 1	-7.92	0.57	-0.32	0.71	-0.59	1.26	5.00	4.00
Event 2	-16.87	0.58	0.83	0.16	0.01	1.00	17.75	-113.00

4.3.1. Flow discharge

Simulation results are displayed in Figure 4.5 to Figure 4.8. Evaluation of these results is presented in Table 4.8. The figures show that flow discharge variations are captured in the model simulation although the variations are very large (e.g. nearly 4 times between the extreme condition and the normal ones). From Table 4.8, it can be seen that the simulated values have a good agreement with observed ones (d index). However, the model performance is still poor when looking at the R², RMSE and NSE values, except the first event. The PBIAS values show that the model overestimates for the first and second events and underestimates for the last events (event 3). Nevertheless, the peaks of flow discharge were well represented. This aspect is very critical since it is assumed that diffuse contaminants are transported during these times.

One reason for above over and under-estimations is the impact of the of rainfall data errors. Data from only one meteorological station was used in this study. Although the catchment is small, its highly topological differences can induce variations of rainfall in time and space, for example by orthographic lifting (Chow et al., 1988, p.64). Event 2 is a clear example of errors in rainfall data. Given observation in the catchment outlet (nearby the rainfall station) that the rain was very heavy (18.6 mm in 2 hours), rainfall observed in a daily rainfall station (Nui Ba station, upstream of the catchment) was only 5 mm. This leads to simulated flood hydrograph which is much higher than the hydrograph induced by rainfall in reality.

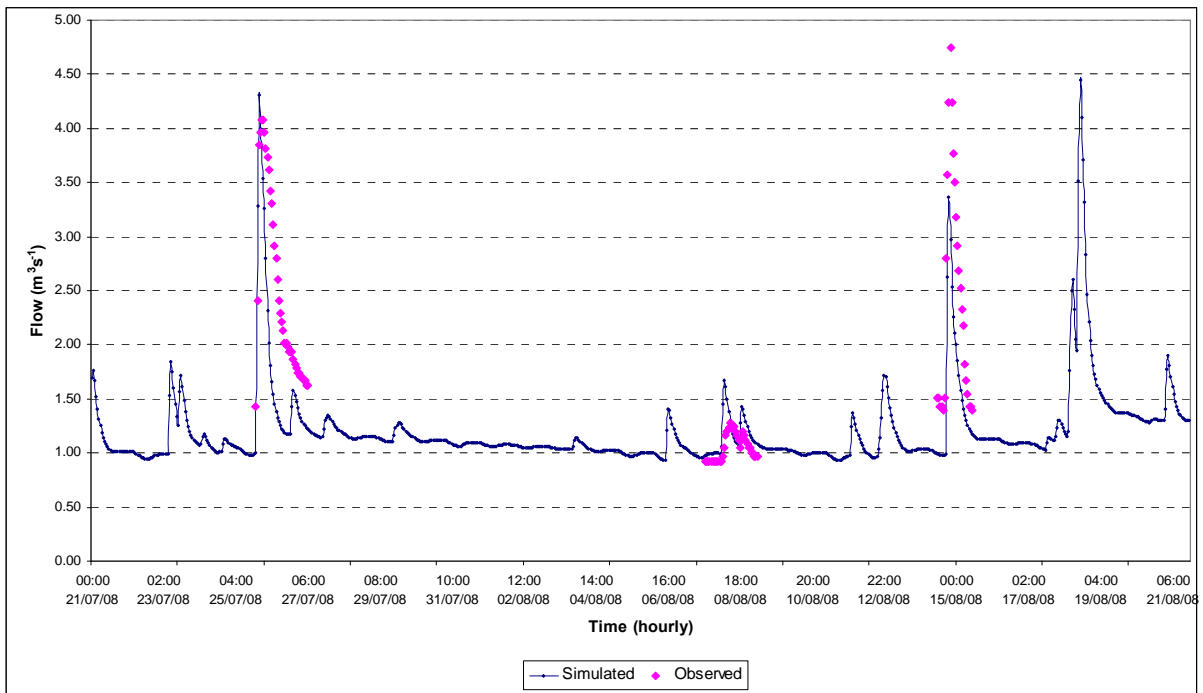


Figure 4.5: Observed and simulated hydrograph from HSPF model (21/7/2008 – 20/8/2008)

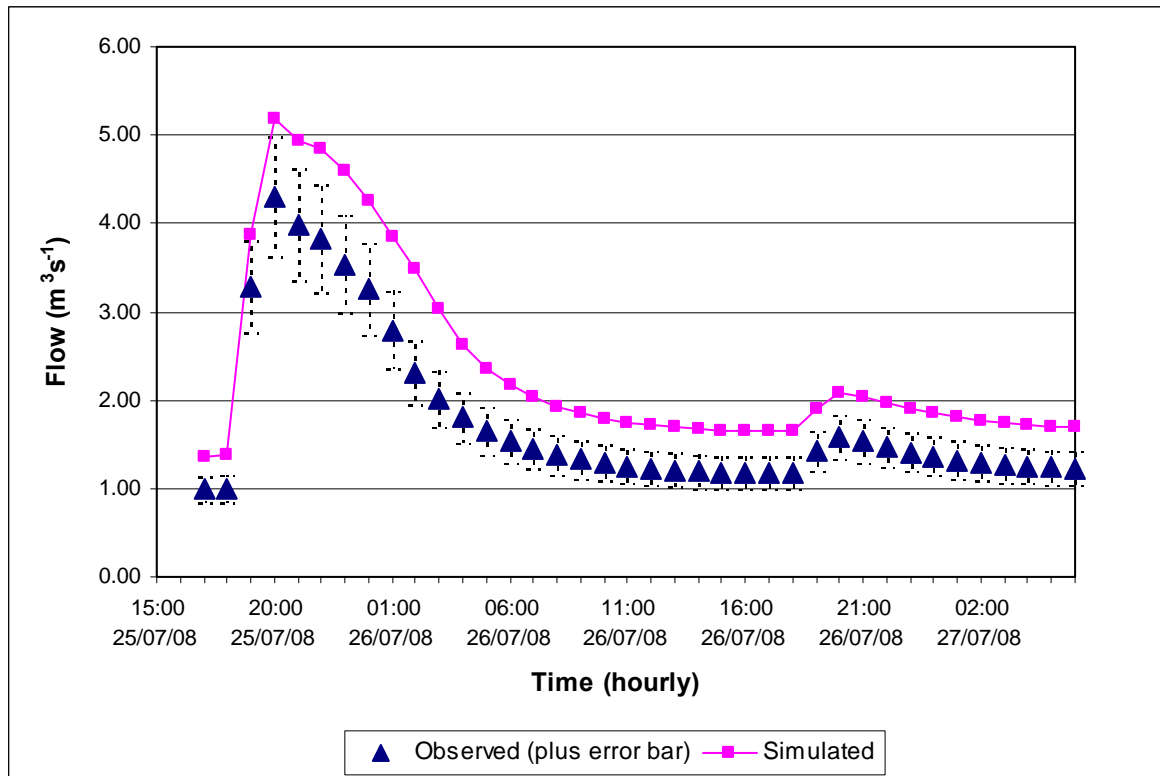


Figure 4.6: Observed and simulated hydrograph from HSPF model (25/7/2008 – 27/7/2008)

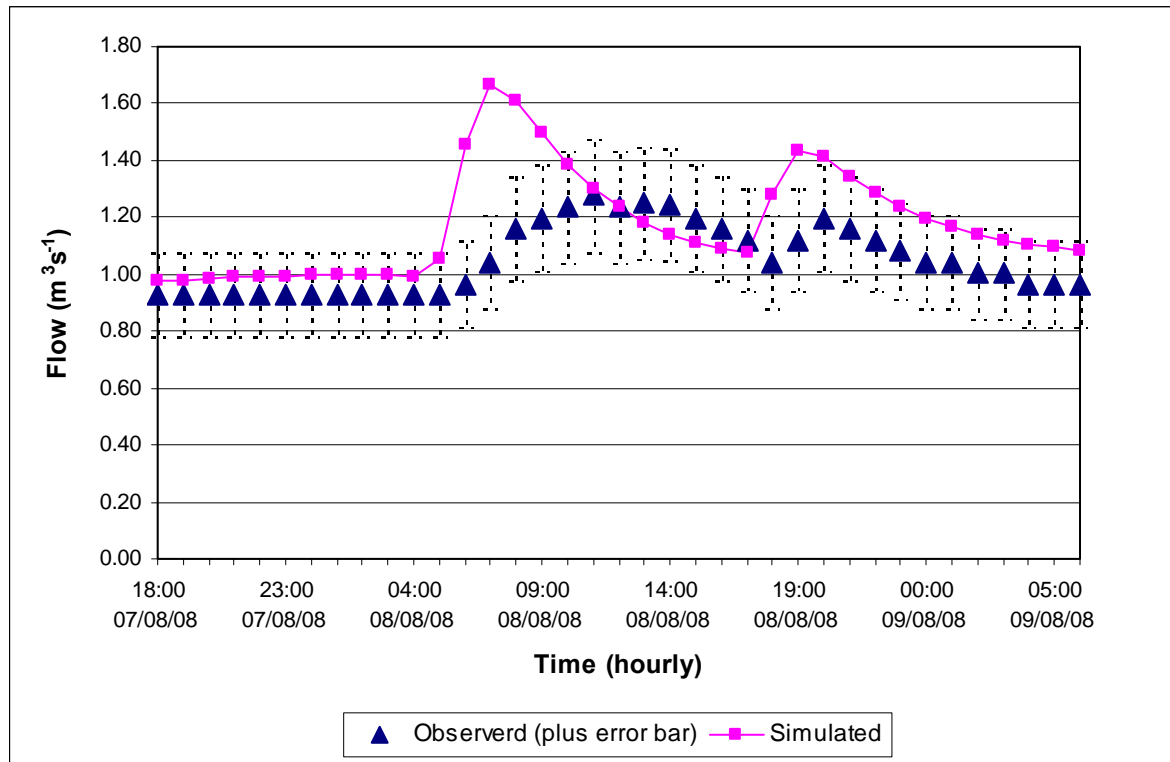


Figure 4.7: Observed and simulated hydrograph from HSPF model (7/8/2008 – 9/8/2008)

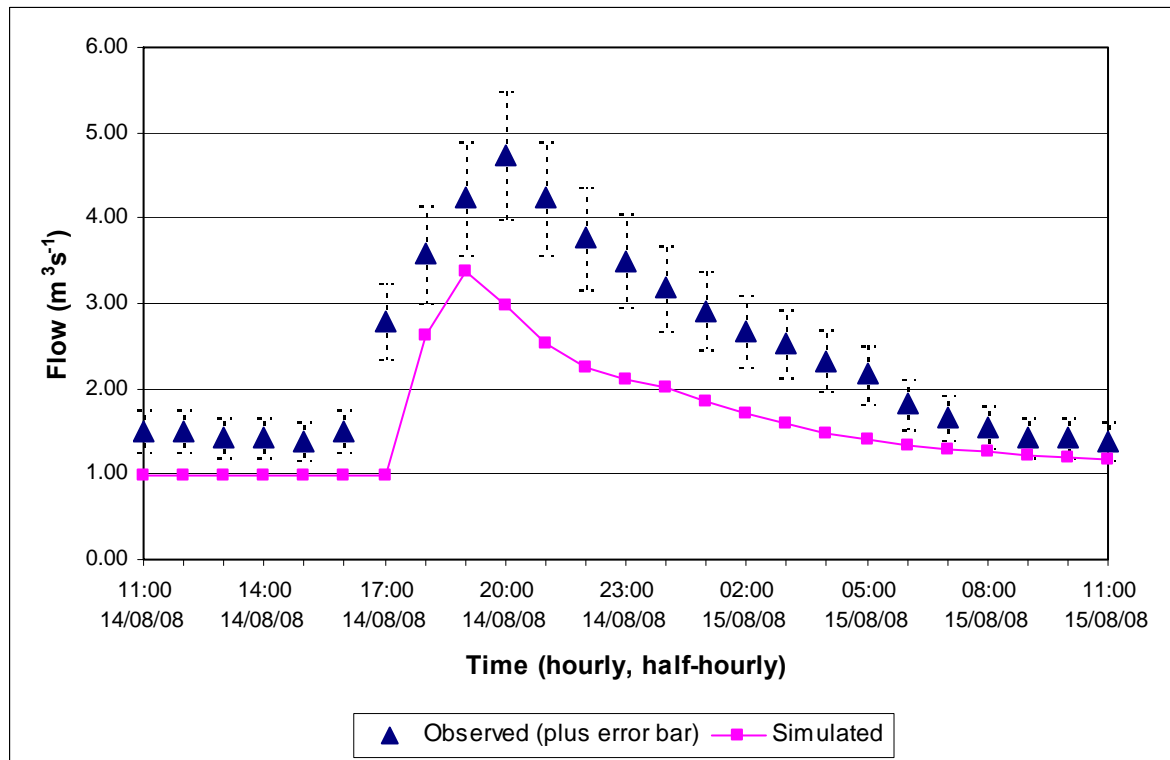


Figure 4.8: Observed and simulated hydrograph from HSPF model (14/8/2008 – 15/8/2008)

4.3.2. Sediment

The simulation results of sediment transport (here is the Total Suspended Solid – TSS) seemed similar to those observed in the flow discharge (see from Figure 4.9 to Figure 4.11). Considering the uncertainties involved in the input data, in the model algorithms and in model parameters, the predicted and observed values have a moderate to good agreement especially during the high flow. However, the model can not reproduce well the observed contaminant during low flow conditions (event 2). In addition, errors caused by from sampling can also contribute to these differences.

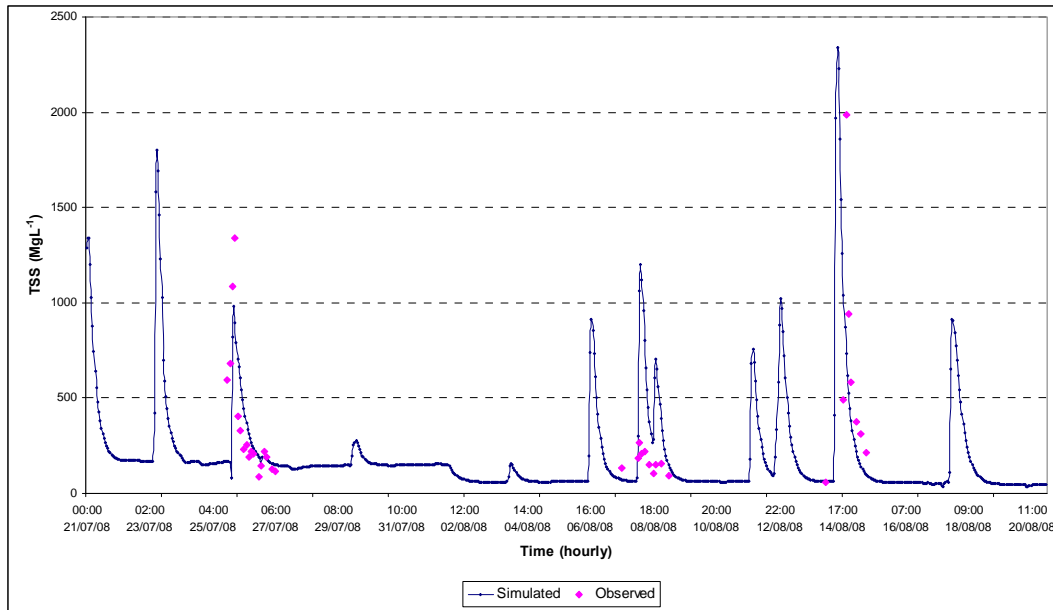


Figure 4.9: Observed and simulated TSS from HSPF model (21/7/2008 – 20/8/2008)

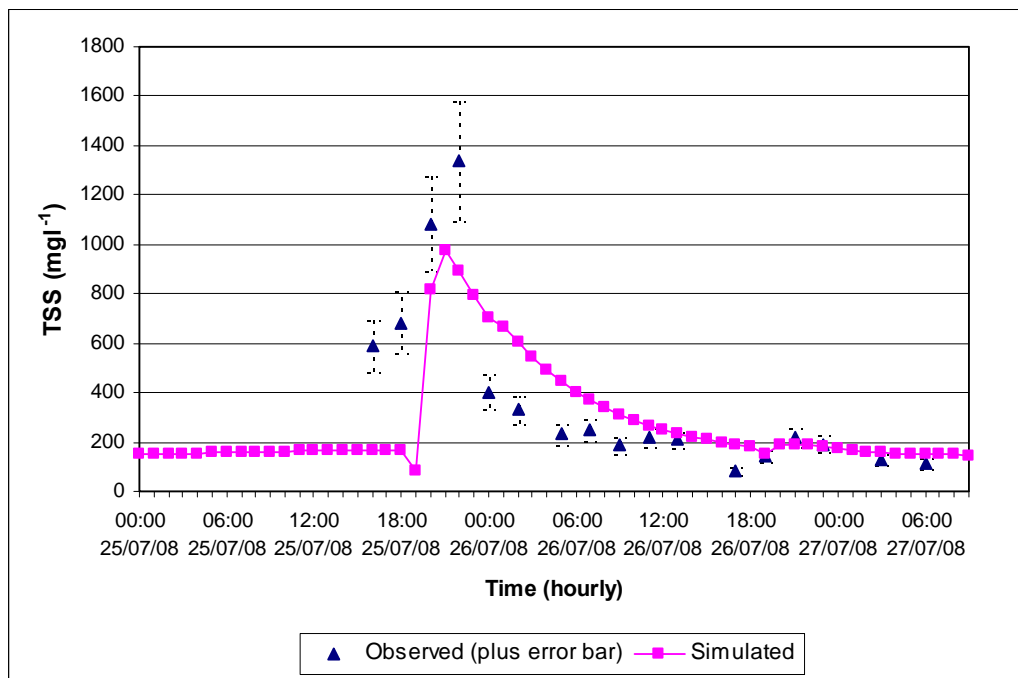


Figure 4.10: Observed and simulated TSS from HSPF model (25/7/2008 – 27/7/2008)

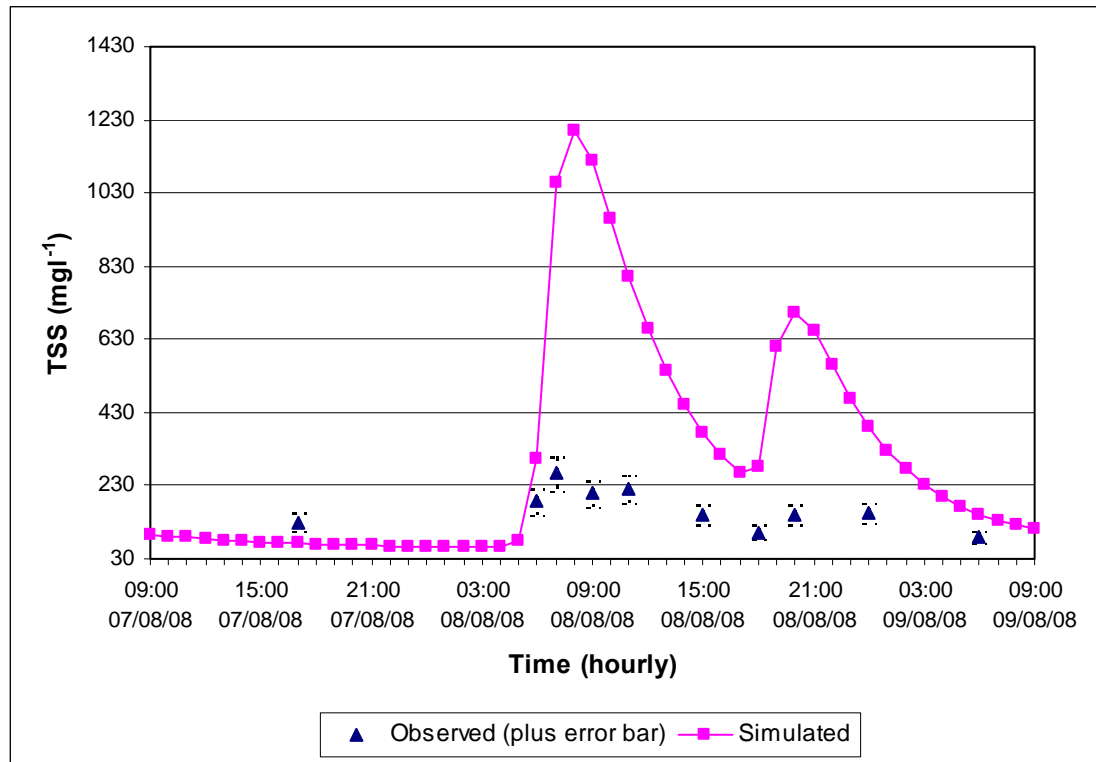


Figure 4.11: Observed and simulated TSS from HSPF model (7/8/2008 – 9/8/2008)

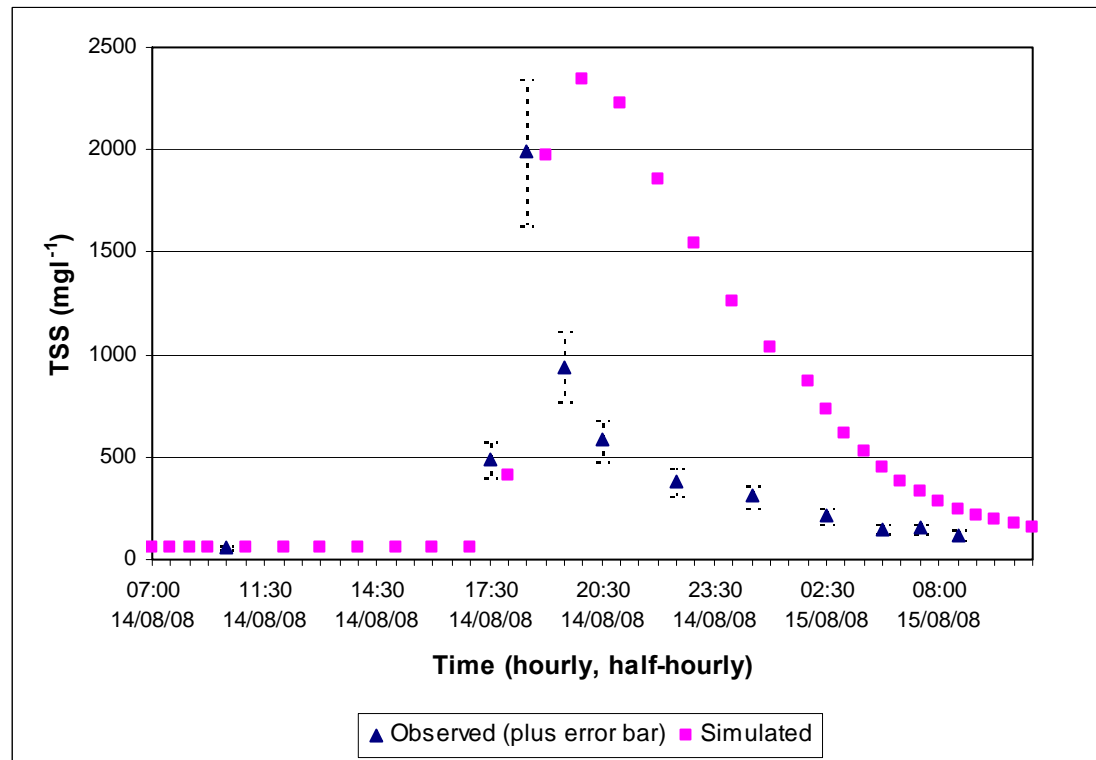


Figure 4.12: Observed and simulated TSS from HSPF model (14/8/2008 – 15/8/2008)

4.3.3. Nutrients

In the first simulation runs, the model could not represent the values observed in the field. Based on own observations in the field (at the tapioca company), it could be possible that the pollutant loadings during the flood events were increased because of the filled-up settling pond or illegal wastewater disposal. Consequently, the input data were modified by increasing wastewater loadings from the company. After several times of “trial”, the model catches the observed nutrient patterns at different magnitudes higher than the normal wastewater loadings. For the first and second events, it was 3, 12 times higher, respectively. In the last event, no point sources since the company closed for renovation.

An example of model results for phosphate phosphorus is shown from Figure 4.13 to Figure 4.16 and Table 4.8; model results for other nutrient parameters (i.e. ammonium, and nitrate) are presented in appendix 4. It is observed that the behaviour of phosphate phosphorus (P-PO₄), aluminium nitrogen (N-NH₄) is quite similar, while nitrate nitrogen (N-NO₃) is different. The N-NO₃ is quite sensitive to flood events, whereas P-PO₄ and N-NH₄ were strongly related to point sources and extreme events only.

With the introduction of “illegal” wastewater disposal, for the first events, only the simulation of P-PO₄ is improved; the simulation of N-NO₃ does not change much; and the simulation of N-NH₄ is even worse. For the second event, the simulation of N-NO₃ has similar behaviour, while the simulation of P-PO₄, N-NH₄ is much improved.

The model adapt very well for simulating the peaks of nutrient variations. However, during the receding flow, the model often underestimates the concentration. This could be explained by retention effects in agricultural fields, especially rice field, where the fields are covered by earth-dykes.

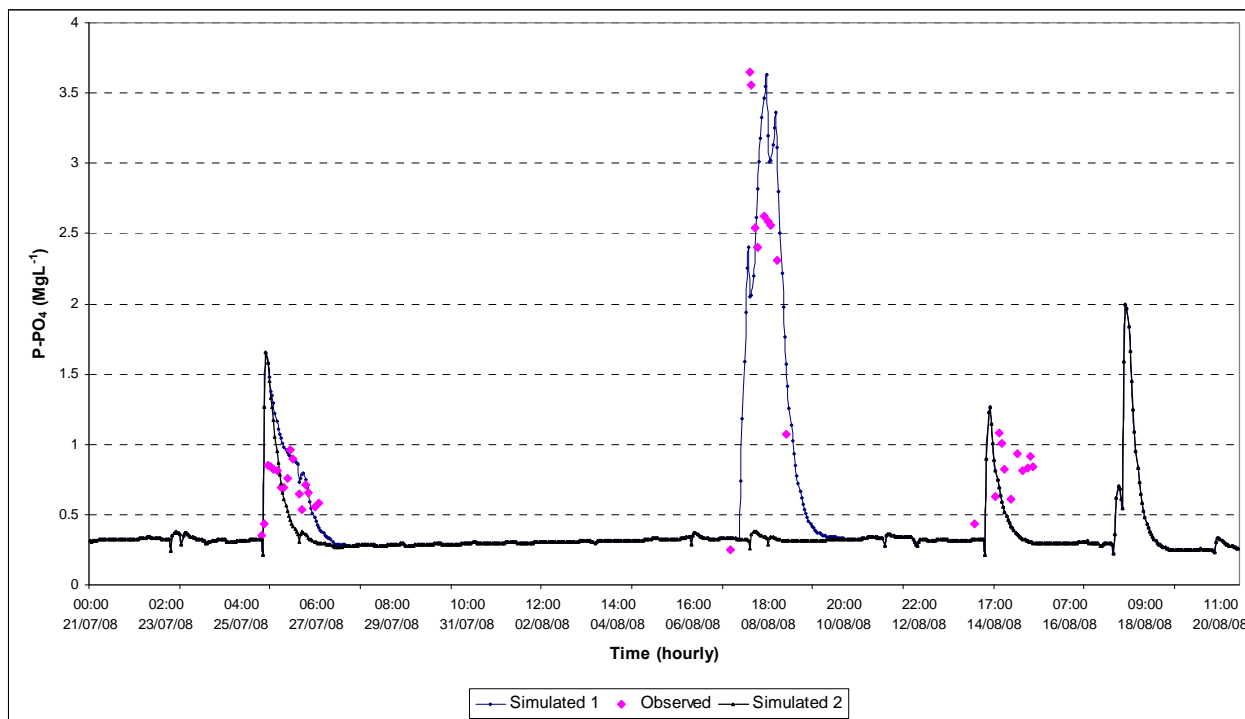


Figure 4.13: Observed and simulated P-PO₄ using HSPF model (21/7/2008 – 20/8/2008)

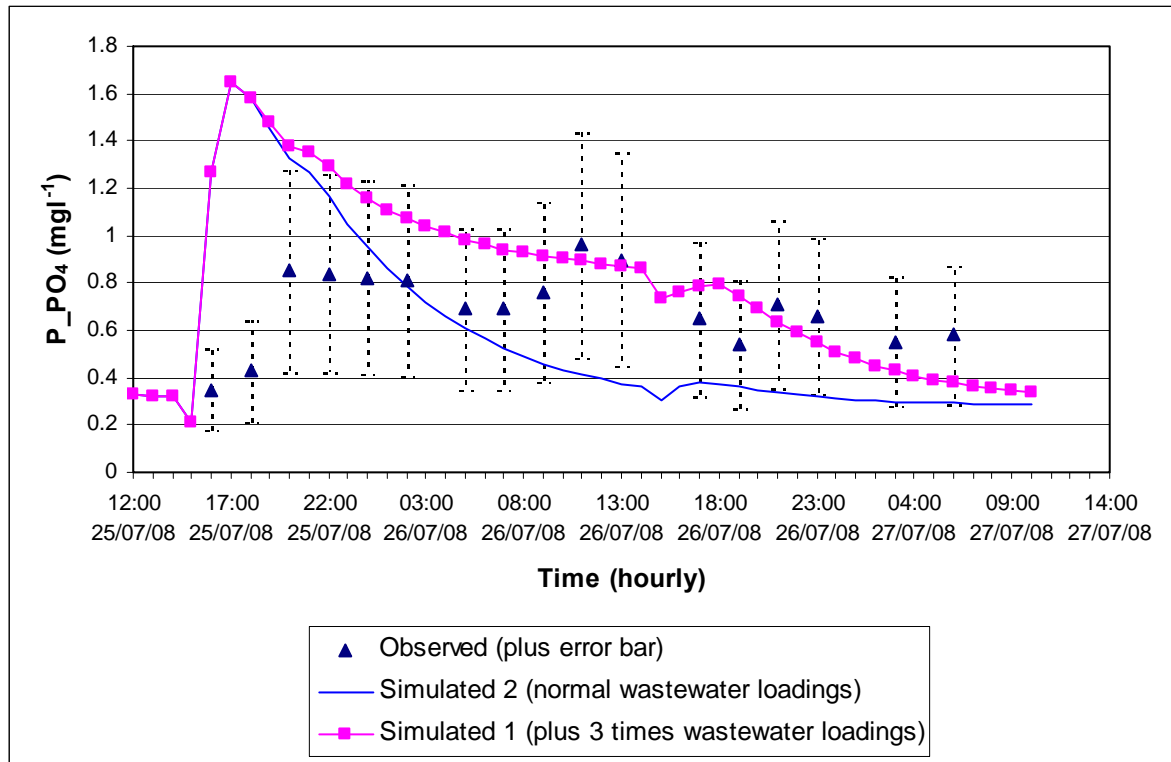


Figure 4.14: Observed and simulated $P\text{-PO}_4$ using HSPF model (25/7/2008 – 27/7/2008)

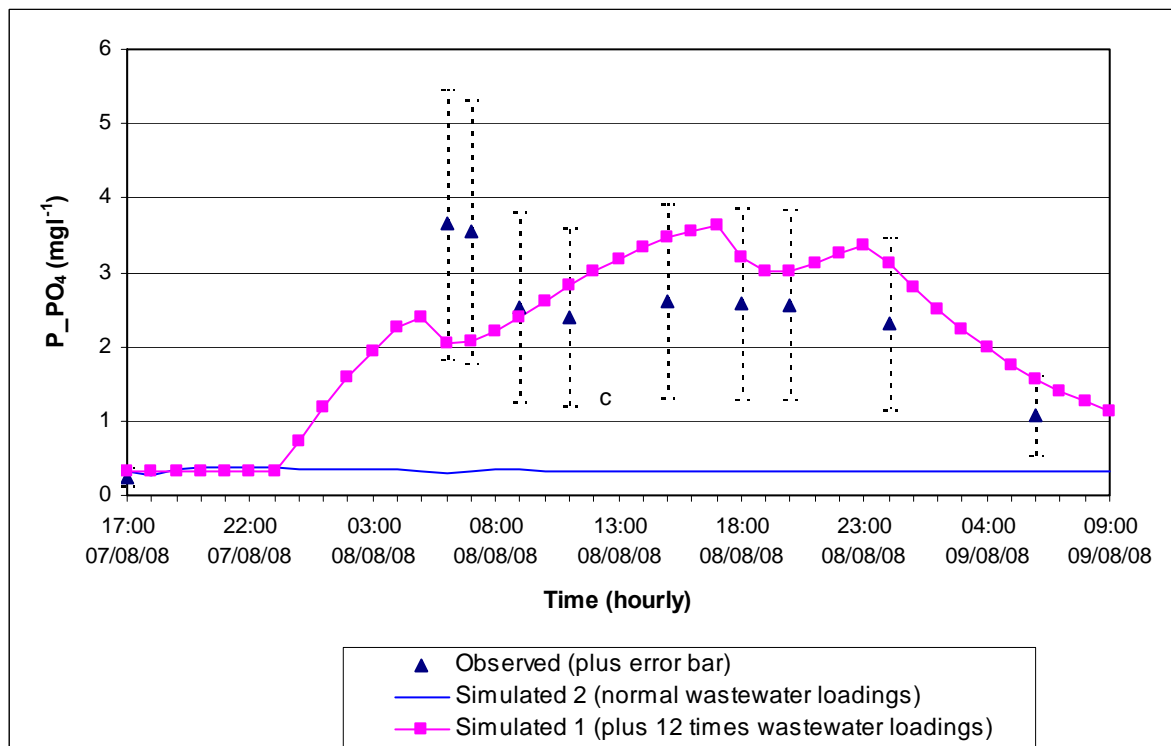


Figure 4.15: Observed and simulated $P\text{-PO}_4$ using HSPF model (7/8/2008 – 9/8/2008)

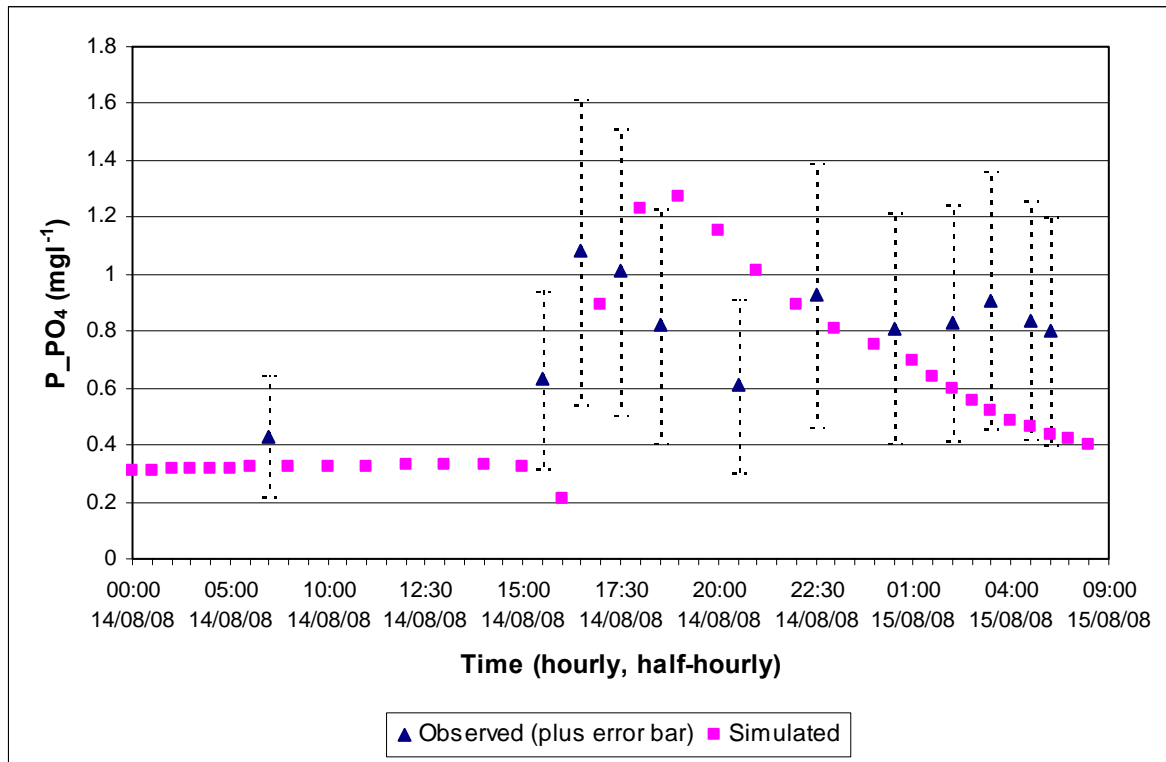


Figure 4.16: Observed and simulated P-PO₄ using HSPF model (14/8/2008 – 15/8/2008)

4.4. Evaluation of HSPF model applications and conclusions

The conclusions for this chapter are given with regard to model preparation and parameterization, model results and model uncertainty.

The calibration for flow discharge and sediment was detailed instructed in the HSPF's user manual and supportive materials and this is relatively straightforward. Most calibrated parameters were within available ranges. However, observed by Radcliffe and Lin (2007) "*Some equations in HSPF are unique to the model, and as a result the parameters for these processes are not readily measured*" that leads to difficulties in reasoning physical senses of model parameters.

Only little guidance for nutrient calibration was found. As a consequence, the results the calibrated parameters are highly site-specific.

Flow discharge and TSS were rather well simulated during high flood events, especially the peaks. Reproduction failed for low flow period. One common reason is because of rainfall data errors. The different rainfall distribution in time and space can lead to over and under-estimation of the real flow by the model

The nutrient dynamics during flood events are well captured by the model. In spite of the abnormal observations, the model was adapted by introducing higher wastewater loadings given the fact that strong smell of tapioca starch wastewater were observed during monitoring, as well as during investigating sewage discharge system of the tapioca company. The abnormal nutrient variation during low flow (event 2) is explainable by considering illegal wastewater disposal (12 times more than normal condition). The improvement of model simulation is clearly seen for phosphate phosphorus and ammonium nitrogen. However, this is not the case for the performance of nitrate nitrogen.

Therefore, it can be concluded that the point sources contribute significantly to phosphate phosphorus and ammonium nitrogen but the diffuse sources control the nitrate nitrogen.

Nutrient dynamics were well simulated during the rising flow; it is not the case during receding flow. This could be an effect of water retention in rice fields where water was released from the after event by farmers in order to keep water level stay at a certain level.

Regarding the *uncertainty* aspects in implementing the HSPF model, several remarks should be kept in mind:

- The model is very complex. Too many parameters can interfere with each other during the calibration processes. Therefore, the problem of equifinality can not be avoided.
- The study catchment can be regarded as ungauged catchment since data is very limited. Many model parameters were estimated from literature (e.g. soil data), not from the real catchment. In addition, input data such as rainfall, pollutant sources (e.g. point sources, nutrient storages in soil – most related to management practice) were also to some extent uncertain. Therefore, for further study (e.g. upscaling), the estimated model parameters have to be checked with care.
- Data is limited for model calibration; no data is available for model validation. Thus, model results for long-term prediction have to be re-assessed by collecting more data. In addition, soil data were not available for a long-term simulation (e.g. several years). The contribution of contaminants from groundwater was ignored in this model application. Thus, the model applied here is limited for short-term simulation of single events.

In conclusion, the comprehensive HSPF model has been successfully implemented. The model can be used for event-based simulations of tropical catchment (extreme events) being exposed to various anthropogenic impacts (point and diffuse sources). The model parameterization is difficult and requires high – level expertise. In addition, given a number of uncertainty sources, especially from model input and model parameters, collecting of more data as well as implementing comparative studies are highly recommended. It became evident, that a simpler and more robust model is required for the simulation of nutrient dynamics during flood events for given tropical condition and a poor database.

5. Model development for nutrient dynamics during flood events – The SINUDYM

5.1. Introduction

As discussed in chapter 2.6.3, there are a number of issues related the development of a modeling system i.e. scaling issues, data limitation (ungauged catchment), model complexity, model uncertainty. In addition, site-specific problems have to be considered. For example, the implementation of the selected HSPF model (among eight popular models) presented in chapter 4 is still limited due to data issues, required expertise and uncertainty sources.

Therefore, objectives of the development of a new model are:

- Compromise between limited data issues and model complexity
- Simple and robust structure to be used for operational purposes
- Easy implementation of uncertainty analysis

In this chapter, firstly, an introduction to the overall modeling framework is presented. In the next sections, detailed descriptions for each component of the framework including rainfall – runoff, erosion/sedimentation, nutrient loadings and river routing are provided as well as how they are parameterized. Model application for one typical event is illustrated in the followed section “simulation results”. Sensitivity analysis and uncertainty analysis are implemented in association with model results in this section. The chapter ends with some discussions on the developed model with regard to its limitations and further improvements.

A model namely SINUDYM which stands for Simplified Nutrient Dynamics Model was developed. A schematic of connected modules within the SINUDYM model is shown in Figure 5.1. A catchment is discretized into a number of sub-catchment. A sub-catchment is considered as a modeling unit for nutrient, sediment generation and transport. In order to capture dominant processes, four model components are considered as follows:

- Hydrology: Runoff after storm events is modelled as a total flow discharge of the catchment. Its results will be later used to convert loadings into concentration at the outlet. Moreover, runoff generated by this hydrological module is used for both sediment and nutrient components.
- Erosion: Soil generation and sediment transport from sources (upland) to receiving water body are simulated at hourly time steps. Results from this module are input to river routing modules.
- Nutrient: In this module, total nutrient loads for each land use types given rainfall and runoff forcing are calculated and then lumped at the sub-catchment outlet. Results from this module are input to river routing modules

- River routing: The transport of nutrient and sediment through a river is routed in the flow routing module. In addition, this module should be able to account for the contribution of point sources (i.e. wastewater discharge from company)

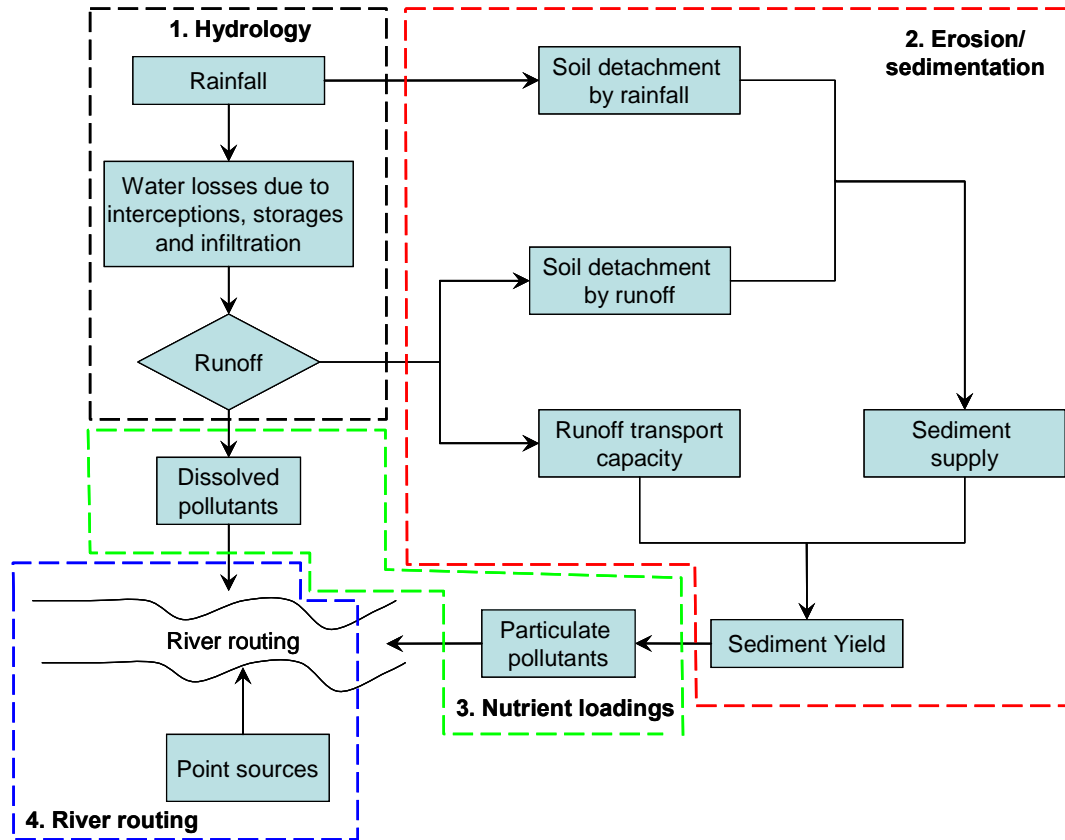


Figure 5.1: Schematic of nutrient transport at sub-catchment scale with model SINUDYM

5.2. Hydrology component

5.2.1. The Geomorphology Instantaneous Unit Hydrograph (GIUH)

The hydrological part is adopted partly from the author's previous works, in which the model had been applied for flood events in Vietnam in 2005 and proved as applicable for the regions (Nguyen, 2006; Nguyen et al., 2009)

The Geomorphology Instantaneous Unit Hydrograph (GIUH) was first initiated by Rodríguez-Iturbe et al. (1979) and restated by Gupta et al. (1980) and it is defined as “**the probability density function of a drop's travel time in a basin**”. Thus, the goal of GIUH theory is to derive this density function based on geomorphologic parameters.

Coupling of quantitative geomorphology and hydrology is at the core of this approach. The model links geomorphological characteristics of a catchment to its response to rainfall (for example relation between hydrograph and topographic factors can be seen in Figure 5.2). In this approach, the Horton's morphometric parameters (Strahler, 1964; Strahler, 1969) including area ratio (R_A), bifurcation ratio (R_B), length ratio (R_L) are mainly used to develop the GIUH.

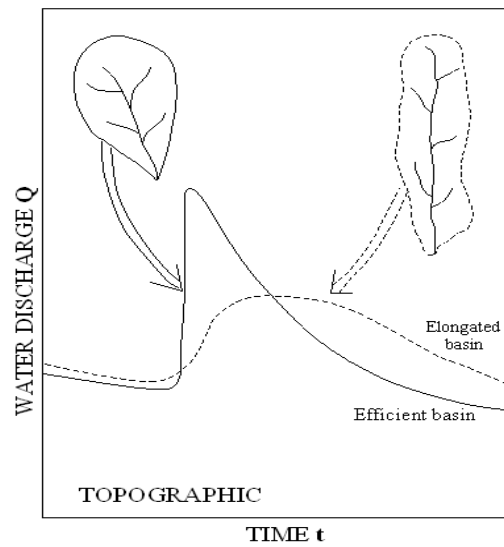


Figure 5.2: Relation between hydrograph and topographic factors (Derbyshire et al., 1981)

In order to determine the GIUH, the input data is considered as rainfall drops which are randomly and uniformly distributed over the catchment. Hereunder, a travel path of one particle is analysed.

The path consists of the route through hillslope areas and channels leading to the outlet. The probability of this water particle follows a certain path among all possible paths from stream of lower order to those of higher order. This order is computed based on the Strahler order scheme. The transition of the drop can be referred to as a change of state. The state is defined as the order of the stream in which a rainfall drop is located at time t . If the rainfall is in a hillslope area, it will drain directly to the stream. After it comes to the stream, it will move to the higher order stream. In another word, the movement of a water particle is a series of transitions from one state to another. From now on, r_i is denoted when the drop is in channel state of order i , and a_i is denoted when the drop is in hillslope state of order i . A catchment has its order ranging from 1 to Ω (Ω is the highest order). A water particle will follow from a point to the catchment outlet through a determined drainage network and hillslope areas. Additionally, it is assumed that only rainfall particles falling on the hillslope areas will be taken into account. Those falling onto streams will be neglected. Given that a particle starts in any one of the hillslope areas, it is governed according to the following rules:

- The only possible transitions out of the state a_i are those of the type $a_i \rightarrow r_i$; $1 \leq i \leq \Omega$:
- The only possible transitions out of the state r_i are $r_i \rightarrow r_j$; $j > i$; $i = 1, 2, \dots, \Omega$:
- A state $r_{\Omega+1}$ is defined as an ending state, and transitions out of $r_{\Omega+1}$ are impossible.

GIUH is an empirical event based model approach that combines easily observable (surface) geomorphologic catchment characteristics with simple regression analysis. The approach is particularly applicable in data scarce areas and model parameterization relies on GIS based DEM processing (Nguyen et al., 2008).

The concept so far has been improved and successfully implemented as an event based hydrological model to simulate rainfall – runoff relation and to forecast floods (Al-Wagdany and Rao, 1998; Nguyen et al., 2009; Rodríguez-Iturbe, 1993; Tuong, 1997). Simulation results showed that the

approach is a very promising tool to estimate event discharges, even for ungauged catchments (Bhaskar et al., 1997; Nguyen et al., 2008).

Rodríguez-Iturbe and Valdez (1979) defined simple empirical relationships for the time to peak (t_{pg}) and the peak flow discharge (q_{pg}) of the GIUH in dependence on geomorphologic parameters

$$q_{pg} = 1.31 R_L^{0.43} \left(\frac{v}{L_\Omega} \right), (\text{hour}^{-1}) \quad (\text{eq. 5.1})$$

$$t_{pg} = 0.44 R_L^{-0.38} \left(\frac{R_B}{R_A} \right)^{0.55} \left(\frac{L_\Omega}{v} \right), (\text{hour}) \quad (\text{eq. 5.2})$$

Where:

- L_Ω = Length of the highest order stream, km
- v = Expected velocity stream flow, m/s
- R_B = Bifurcation ratio
- R_A = Area ratio
- R_L = Length ratio

In equations (1), (2) the geomorphologic parameters (R_B , R_A , R_L) can easily be extracted based on the topological characteristics of the catchment using GIS e.g. ILWIS (ITC, 2001). The flow velocity has to be defined by physical reasoning where an average velocity must be related to some average flow length (i.e. travel path) and travel times.

The response function of the GIUH is characterised as an “*impulse response function*”. If a system receives an input of unit amount applied instantaneous (a unit impulse) at time τ , the response of the system at a later time t is described by the unit impulse response function $u(t-\tau)$, $t-\tau$ is the time lag since the impulse is applied (Chow et al., 1988, p.204). The amount of input entering the system between time τ and $\tau + d\tau$ is $i(\tau)d\tau$. If $i(\tau)$ is the effective rainfall, the response of a complete input $i(\tau)$ is the direct runoff $Q(t)$ of the catchment. This runoff can be found by integrating the response to its constituent impulse (convolution integral) as:

$$Q(t) = \int_0^t i(\tau)u(t-\tau) \quad (\text{eq. 5.3})$$

Where:

- $i(t)$ = Effective rainfall intensity, and distributed uniformly over the entire basin
- $u(t)$ = The GIUH in this case

The effective (excess) rainfall is computed according to the Soil Conservation Service (SCS) runoff method (Chow et al., 1988; Ogrosky and Mockus, 1964)

5.2.2. Model development

In order to implement the GIUH, data needed include:

- **DEM** used to derive the Horton’s morphometric parameters
- **Land cover** and **soil** data used to estimate the curve number (CN) value when applying SCS method.

- **Rainfall** used as input of the model
- **Discharge** used as references of the output of the model i.e. model calibration

5.2.2.1. The GIUH parameterization

The channel network of a catchment reflects the relationship of hillslopes and channels. This pattern is represented in a GIUH model in a probabilistic sense. The GIUH is interpreted as the probability density function of the travel times to the outlet of the rain randomly, uniformly distributed over the catchment. The travel times on hillslope or along streams are assumed exponentially distributed. The probabilities including the initial probability and transition probability are calculated based on Horton's morphometric parameters. The parameters are bifurcation ratio (R_B), length ratio (R_L) and area ratio (R_A). Using Strahler's ordering scheme (Strahler, 1969), the ratios can be expressed quantitatively as shown in Table 5.1

Table 5.1: Horton's ratios

Ratios	Formula	Notes
Bifurcation	$R_B = \frac{N_i}{N_{i+1}}$	where N_i and N_{i+1} are the number of streams in order i and $i+1$. Let Ω represent the highest stream order in catchment, $i = 1, 2, \dots, \Omega$.
Length	$R_L = \frac{\bar{L}_{i+1}}{\bar{L}_i}$	\bar{L}_i is average length of channels of order i is: $\bar{L}_i = \frac{1}{N_i} \sum_{j=1}^{N_i} L_{j,i}$
Area	$R_A = \frac{\bar{A}_{i+1}}{\bar{A}_i}$	\bar{A}_i is the mean area of the contributing sub-catchment to streams of order i , $\bar{A}_i = \frac{1}{N_i} \sum_{j=1}^{N_i} A_{j,i}$, where $A_{j,i}$ represents the total area that drains into the j^{th} stream of order i

The R_B , R_L and R_A values vary normally between 3 and 5 for R_B , between 1.5 and 3.5 for R_L and between 3 and 6 for R_A (Rodríguez-Iturbe, 1993, p.45).

This concept can be explained through a deterministic way of routing through linear reservoirs (Chutha and Dooge, 1990) as illustrated by Figure 5.3. The θ_i , p_{ij} , λ_i , in this figure are initial probabilities, transition probabilities, mean travel time, respectively. The initial probability accounts for a drop falling to any hillslope¹² areas in the catchment either in 1st, 2nd or 3rd catchments (represented by θ_1 , θ_2 , θ_3). The transition probability then accounts for the changing stage of a drop from low order stream to the higher ones. For example at the 1st order stream, the drop can either go to 2nd order or 3rd order (represented by p_{12} and p_{13}). The mean travel time accounts for any stage. It includes travel time from hillslope to stream and along all of streams. The next paragraph will explain how to derive the GIUH as well as how to calculate these parameters.

¹² Rainfall falls to the channel network is neglected.

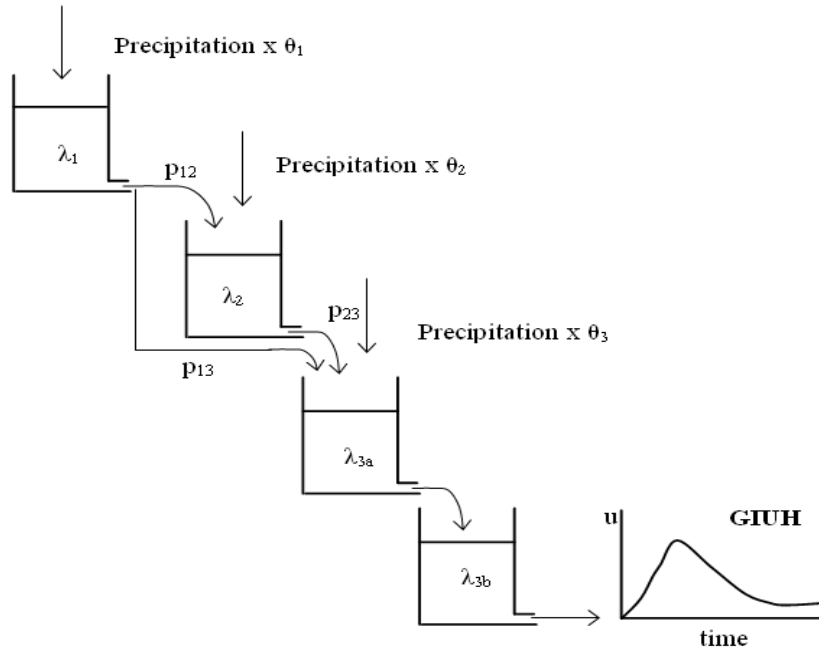


Figure 5.3: Representation of a third – order basin as a combination of linear storage in parallel and in series (Franchini and O'Connell, 1996)

The GIUH is the *impulse response function* of the system, now denoted as $u(t)$, is determined as following:

$$u(t) = \frac{\partial}{\partial t} \text{Prob}(T_B \leq t) \text{ or: } u(t) = \frac{\partial}{\partial t} \left(\sum_{S_i} \text{Prob}(T_{S_i} \leq t) \text{Prob}(S_i) \right) \quad (\text{eq. 5.4})$$

Where:

- Prob() = Stands for the probability of the set given in parenthesis;
- T_B = The time of travel to the catchment outlet;
- T_{S_i} = The travel time in a particular path;
- Prob(S_i) = The probability of a drop which will travel all possible paths S_i to the outlet
- $\text{Prob}(T_{S_i})$ = The probability density function (pdf) of the total path travel time T_{S_i} .

For the 3rd order catchment, the possible paths S_i of water are:

- Path S_1 : $a_1 \rightarrow r_1 \rightarrow r_2 \rightarrow r_3 \rightarrow \text{outlet}$;
- Path S_2 : $a_1 \rightarrow r_1 \rightarrow r_3 \rightarrow \text{outlet}$;
- Path S_3 : $a_2 \rightarrow r_2 \rightarrow r_3 \rightarrow \text{outlet}$;
- Path S_4 : $a_3 \rightarrow r_3 \rightarrow \text{outlet}$.

(a_i is denoted when the drop in hillslope state of order i , and r_i is denoted when the drop in channel state of order i)

And the probability of any path is,

$$\text{Prob}(S_i) = \theta_j p_{ij} p_{jk} \dots p_{l\Omega} \quad (\text{eq. 5.5})$$

Where:

θ_j = The initial state probabilities

p_{ij} = The transition probabilities¹³

$$\theta_j = \frac{(\text{total area draining directly into streams of order } i)}{(\text{total catchment area})}$$

$$p_{ij} = \frac{(\text{number of streams of order } i \text{ draining into streams of order } j)}{(\text{total number of streams of order } i)}$$

The travel time T_s , in a particular path must be equal to the sum of travel times in the elements of that path.

$$T(S_i) = T_{ai} + T_{ri} + T_{ri+1} + \dots + T_{r\Omega} \quad (\text{eq. 5.6})$$

Where:

T_{aj} = The travel time on the hillslope

T_{ri} = The travel times in each stream segment of order i ($1 \leq i \leq \Omega$, Ω is the highest order)

Assuming that these individual times of travel are independent variables such that f_{Ta} is the pdf of T_{aj} , f_{Tr} is the pdf of T_{ri} , and that f_{Si} is pdf path S_i , the probability of the sum, T_{Si} , is a multiple convolution integral of the following form:

$$\text{Prob}(T_{Si}) = \sum_{s \in S} f_{Si}(t) = \sum_{s \in S} f_{Tai}(t) f_{Tri}(t) f_{Tri+1}(t) \dots f_{Tr\Omega}(t) \quad (\text{eq. 5.7})$$

Where:

$f_{Tai}(t)$ = $f_{Tai}(t) = \alpha_i \exp(-\alpha_i t)$, is a gamma function corresponding to the travel time of a drop in a given hillslope that obeys the exponential probability density function.

$f_{Tri}(t)$ = $f_{Tri}(t) = \beta_i \exp(-\beta_i t)$, is a gamma function corresponding to the travel time of a drop in a given channel that obeys the exponential probability density function.

The α , β is mean travel time for hillslope and for stream flow respectively, and v is expressed by v_o for hillslope velocity and v_s for stream velocity, respectively.

$$\beta_i = \frac{v}{\bar{L}_i}, \quad \alpha_i = \frac{v}{L_o}, \quad L_o = \frac{1}{2D}, \quad \text{is average overland flow and } D \text{ is drainage density}$$

The α_i is kept constant for any given hillslope ($\alpha_1 = \alpha_2 = \alpha_3$), while the β_i is changed according to the average length of each given order stream (\bar{L}_i).

Then the GIUH, $u(t)$ is computed as:

$$u(t) = \sum_{s \in S} f_{Tai}(t) \times f_{Tri}(t) \times f_{Tri+1}(t) \times \dots \times f_{Tr\Omega}(t) \times \text{Prob}(S) \quad (\text{eq. 5.8})$$

¹³ Formula to calculate is shown in appendix 5

This formula is solved in hourly time step using the Microsoft Excel spread sheet.

Model parameters of the GIUH include the Horton's ratios, hillslope and stream flow velocity. The estimated flow velocity will be included in the result part (section 5.6), hereunder the method to derive the Horton's morphologic parameter.

The Horton's statistics including R_A , R_L , R_B are calculated using a new functionality in ILWIS called "*Horton statistics*" in module "*statistical parameter extraction*" (in "**DEM – Hydro-processing**") (Maathuis and Wang, 2006). The process is as follows:

- Calculating the number of streams, the average stream length (km), and the average area of catchments (km²) for all streams. (Represented by C_N , C_L , C_A in Table 5.2).
- Calculating expected values of the number of streams, the average stream length (km), the average area of catchments (km²) by means of a least squares fit. (Represented by C_{N_LSq} , C_{L_LSq} , C_{A_LSq} in Table 5.2)
- The R_A , R_L , R_B are the slope of each fitted line connecting the expected values shown in Figure 5.4 (result shown in Table 5.2);

The obtained values and the least square fit are visualized using a Horton plot to inspect the regularity of the extracted stream network and serve as a quality control indicator for the entire stream network extraction process. It is expected that (Strahler, 1964):

- The number of streams show a decrease for subsequent higher order Strahler numbers;
- The length of streams and the catchment areas show an increase for subsequent higher order Strahler numbers.

From the Horton plot (Figure 5.4) and the Table 5.2 it can be assessed that the drainage network is well extracted, that the Horton number are representative and fall within the expected range and used without calibration. The extracted river network is presented in Figure 3.4.

Table 5.2: Values of number of streams, the average stream length, and the average area, their expected values and the Horton's ratios

Order	C1_N (number)	C1_L (km)	C1_A (km ²)	C1_N_LSq (number)	C1_L_LSq (km)	C1_A_LSq (km ²)	Horton's Ratio		
							RB	RL	RA
1	8	2.2	1.31	7.127	2.556	1.639	2.83	1.83	4.00
2	2	6.31	10.26	2.52	4.673	6.555			
3	1	7.35	20.96	0.891	8.541	26.221			

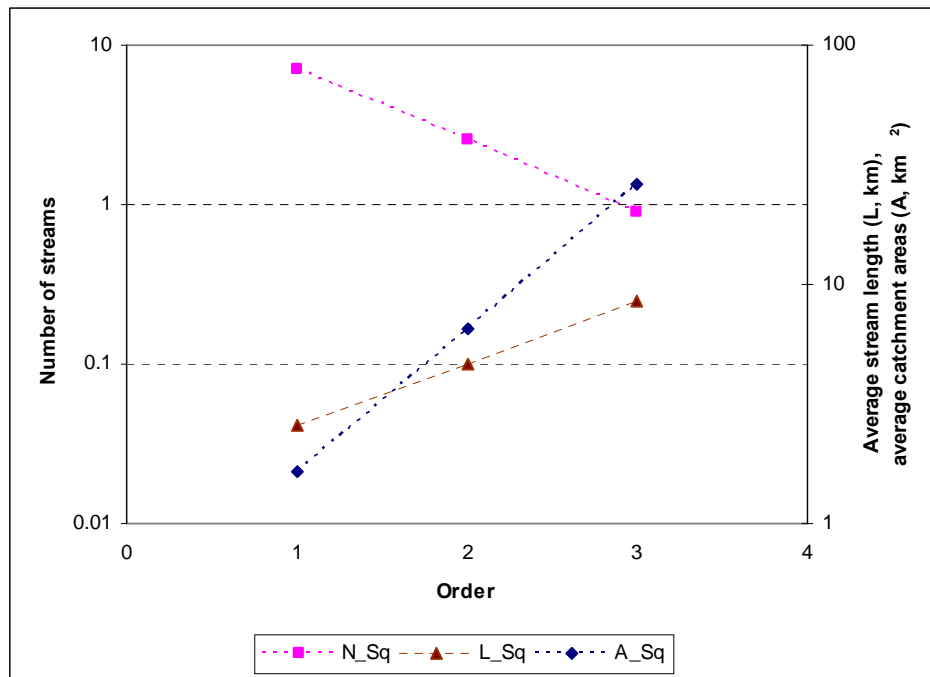


Figure 5.4: Regression of logarithm of the number of streams, average stream length, average catchment area for the Tra Phi catchment

5.2.2.2. Surface discharge calculation based on GIUH

The above section “GIUH development” has shown how to derive the GIUH; in the following part, the calculation of the surface discharge for each event is described.

The effective (excess) rainfall is computed according to the Soil Conservation Service (SCS) runoff method (see Ogrosky and Mockus, 1964 for original) and (Chow et al., 1988, p.147 for latest one). To calculate the Curve Number (CN) value, the land use map and soil map are used based on the SCS table. The CN values of each map unit are aggregated for the whole catchment by means of GIS to get an average CN value (e.g. see in Nguyen, 2006). Then direct flow or the effective rainfall is calculated using the equation eq.2.3

After having the effective rainfall, Horton’s statistics values to derive GIUH, the surface runoff is calculated (see Chow et al., 1988, p.211) and the discharge is determined by taking into account the catchment area.

5.2.2.3. Base flow separation

The catchment flow is composed of three components which are assumed to occur separately and simultaneously. As illustrated in the hydrograph which is constituted by rising limb and recession limb. The components include: (1) surface flow (overland flow), (2) subsurface runoff, or interflow and (3) base flow or groundwater flow. In the GIUH approach, the model can basically simulate the overland flow plus parts of the interflow which leave the unsaturated zone and arrive as surface flow at the river. So, from the observed hydrograph, the contribution of base flow need to be subtracted.

In this study, the base flow is separated manually using the constant slope method (McCuen, 1998); result for a flood event 25-26 July 2008 is showed in Figure 5.5

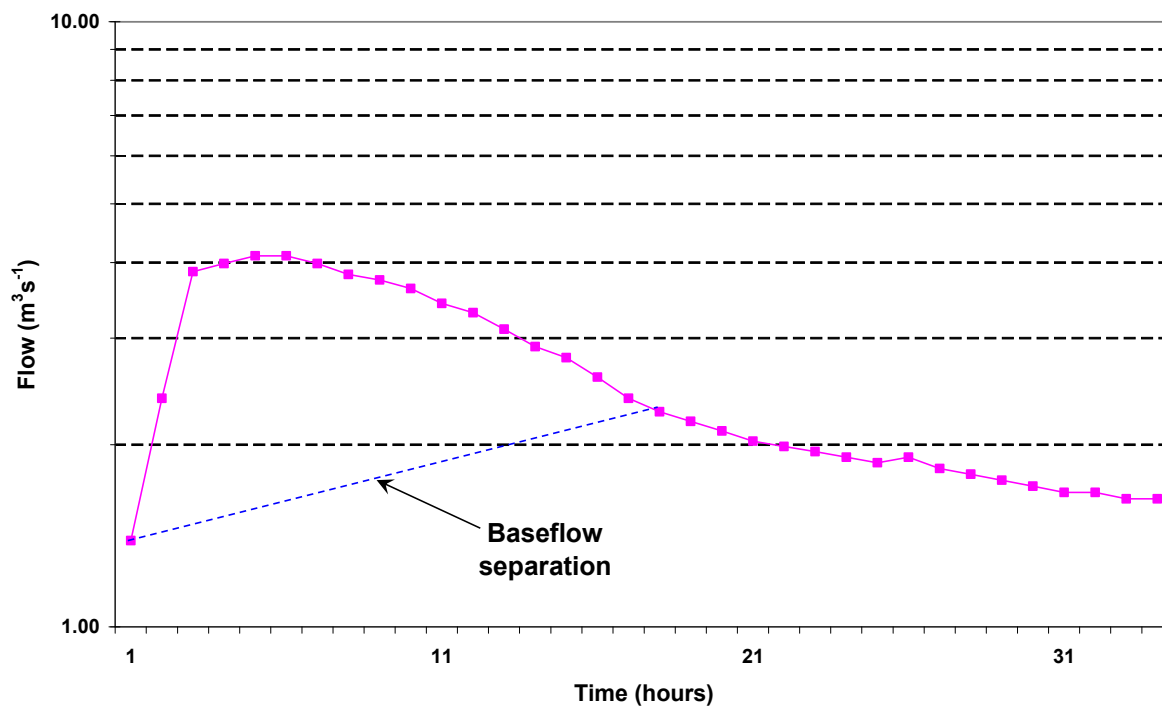


Figure 5.5: Baseflow separation for flood event 25-26 July 2008

5.3. Erosion/sediment component

5.3.1. The simplified process model for sediment yield

5.3.1.1. Introduction

The erosion/sediment component was developed based on simplified process (SP) model for sediment yield which is basically adapted from *Hartley (1987a)*. The model was tested and is proved to be suitable for modeling erosion during (extreme) flood events at hourly time step (*Hartley, 1987b; León et al., 2001*). The model attempted to “*minimize both data inputs and computational effort while maintaining a relatively high degree of similitude with both hydrologic and hydraulic processes*” (*Hartley, 1987a*). The erosion model aimed to compromise between the simple empirical modeling approach, e.g. the USLE, and the complex physically-based one, e.g. KNIEROS (*Hartley, 1987a*).

A schematic of the model was presented in module “erosion/sedimentation” of Figure 5.1. Basically, sediment supply is the sum of sediment detached by runoff and sediment detached by rainfall. Runoff is the only source for transporting sediment which is represented by “sediment transport capacity”. The runoff is calculated from the hydrological component. After comparing the “sediment supply” and “sediment transport capacity”, the smaller is the “sediment yield” from the catchment.

5.3.1.2. Model algorithms

a. Sediment supply

The potential sediment supply caused by rainfall is calculated based on the rainfall energy rate which is used in the USLE method, whereas caused by runoff is upon the stream power equation.

Sediment detached by rainfall

Sediment supply by rainfall is calculated as follows:

$$G_{rf} = E_{rf}(1 - GC)CF \times D \quad (\text{eq. 5.9})$$

Where:

- G_{rf} = Rate of soil detachment due to rainfall (mass rate of detachment per unit area by rainfall) $\text{kg/m}^2/\text{h}$
- E_{rf} = Rate of rainfall energy (rainfall power per unit area) $(\text{J/m}^2/\text{h})$, kg/h^3
- GC = Ground cover factor, see Table A6.1, Appendix 6
- CF = Canopy factor (-), C value in USLE method, section 2.2.2.1, chapter 2, table A6.1 Appendix 6
- D = Soil erodibility factor (kg/J) , (h^2/m^2) , K value in USLE method, section 2.2.2.1., chapter 2, table A6.2 Appendix 6

The rate of rainfall energy is:

$$E_{rf} = i(11.9 + 8.7 \log_{10} i) \quad (\text{eq. 5.10})$$

Where:

- i = Rainfall (mm/h)

Sediment detached by runoff

Sediment supply by runoff is calculated as follows:

$$G_{ro} = E_{ro}D \quad (\text{eq. 5.11})$$

Where:

- G_{ro} = Rate of soil detachment due to runoff (mass rate of detachment per unit area by runoff) $(\text{kg/m}^2/\text{h})$
- E_{ro} = Runoff power per unit area) rate of energy input to the soil by the flow $(\text{J/m}^2/\text{h})$, (kg/h^3)
- D = Soil erodibility factor, kg/J , h^2/m^2 , K value in USLE method, section 2.2.2.1, chapter 2, table A6.2 Appendix 6

The rate of runoff energy is:

$$E_{ro} = \left(\frac{60}{K_f} \right) \gamma \frac{Q_L}{2} S_0 \quad (\text{eq. 5.12})$$

Where:

- K_f = Overland flow resistance (overland flow friction parameter, relating to ground cover density, e.g. $K_f=130.3$)
- γ = Water specific weight $(\text{kg/m}^2/\text{s}^2)$
- Q_L = Unit flow discharge (m^2/h)
- S_0 = Element slope (-)

The unit flow discharge is calculated according to the algorithm presented in Chow et al. (1988, p.156):

$$Q_L = r \times L_0 \times \cos(\theta) \quad (\text{eq. 5.13})$$

Where:

$$\begin{aligned} r &= \text{Runoff, m} \\ L_0 &= \text{Used as overland flow length in this model} \\ L_0 &= \frac{1}{2D} \\ D &= \text{Drainage density, m/km} \\ \theta &= \text{Slope angle} \end{aligned}$$

Thus the potential sediment supply (Y_S) within time duration (Δt) is:

$$Y_S = (G_{rf} + G_{ro}) \Delta t \quad (\text{eq. 5.14})$$

b. Sediment transport capacity

The transport capacity is based on a sediment concentration ratio estimated with a shear stress relationship between the dominant flow shear on the soil and the critical stress based on the Shields criteria (Simons and Senturk, 1976, cited in Hartley, 1987a).

The sediment transport capacity (Y_C):

$$Y_C = 2.65 \rho c r \quad (\text{eq. 5.15})$$

Where:

$$\begin{aligned} \rho &= \text{Density of water, kg/m}^3 \\ c &= \text{Sediment concentration ratio} \\ r &= \text{Runoff, m} \end{aligned}$$

The sediment concentration ratio:

$$c = A \left(\frac{\tau_s}{\tau_c} \right)^B \quad (\text{eq. 5.16})$$

Where:

$$\begin{aligned} A &= \text{Coefficient in transport capacity relationship (A=0.00066)} \\ B &= \text{Power in transport capacity relationship (B=1.61)} \\ \tau_s &= \text{Shear stress on the soil (kg/m/h}^2\text{)} \\ \tau_c &= \text{Critical shear stress (kg/m/h}^2\text{)} \end{aligned}$$

The shear stress τ_s varies both in space and time during a runoff event on the surface. For the sake of simplicity it is proposed to define a single, mean or “dominant” shear stress for an entire runoff event from a given surface (Hartley, 1987a), that means τ_s is equal to τ_D

Dominant flow shear stress:

$$\tau_D = \frac{\beta}{\beta + 1} \left(\frac{60}{K_f} \right) \gamma \bar{h}_L S_0 \quad (\text{eq. 5.17})$$

Where:

$$\begin{aligned} \beta &= \text{Power in the depth-discharge relationship parameter (=5/3)} \\ \bar{h}_L &= \text{Time average runoff flow depth (mm)} \end{aligned}$$

The time average runoff is calculated based on the kinematic approximation:

$$\bar{h}_L = \left(\frac{Q_L}{\alpha} \right)^{\frac{1}{\beta}} \quad (\text{eq. 5.18})$$

Where:

$$\begin{aligned} \alpha &= \text{Coefficient in the depth-discharge relationship} \\ \alpha &= \left[\frac{8gS_0}{0.0074K_f\nu^{0.25}} \right]^{0.57} \\ g &= \text{Gravity coefficient, m/s}^2 \\ \nu &= \text{Kinematic viscosity of water, } =10^{-6}, \text{ m}^2/\text{s} \end{aligned}$$

Critical shear stress:

$$\tau_C = (\sigma - 1) \left(\frac{60}{K_f} \right) \gamma \phi D_{50} \quad (\text{eq. 5.19})$$

Where:

$$\begin{aligned} \sigma &= \text{Specific weight of sediment (-), table A6.2 Appendix 6 (as SpG)} \\ \phi &= \text{Shield sediment function (-)} \\ D_{50} &= \text{Median size of soil particle (mm), table A6.2 Appendix 6} \end{aligned}$$

Shields entrainment function:

$$\phi = \frac{0.11}{R^*} + 0.021 \log_{10} R^* \quad (\text{eq. 5.20})$$

Where:

$$R^* = \text{Shield criterion Reynold number (-)}$$

Shield criterion Reynolds number:

$$R^* = \frac{\sqrt{\frac{\tau_D}{\rho}} D_{50}}{\nu} \quad (\text{eq. 5.21})$$

Since water samples were collected in surface water, it is assumed only clay sediment was collected. Predicted sediment in the model, therefore, should be clay. In this approach, the clay fraction (Fcl) in sediment calculated based on the approach presented in Table 2.2 (chapter 2) is adapted.

$$Fcl = 0.26 \times Ocl$$

Where:

Fcl = Clay fraction in detached sediment

Ocl = Clay fraction in matrix soil (0.04 for Acrisol)

5.3.2. Model setup (development)

The development of the erosion/sediment yield model includes 4 main steps:

- Extracting runoff values from hydrological model
- Calculating soil detachment by runoff and soil detachment by rainfall
- Calculating sediment transport capacity
- Calculating sediment yield

5.3.2.1. Data requirement

In section 5.3.1.2, there are a number of model parameters related to soil, catchment characteristics, rainfall, and runoff are described. Specifically, they are: (1) Soil data: Median size of soil particle (D_{50}), specific weight of sediment (σ), soil erodibility factor (D); (2) Land use data: ground cover factor (GC), canopy factor (GF); (3) Physical characteristics of catchment: slope (S_o), catchment areas, overlandflow length (L)

5.3.2.2. Model parameterization

Model parameters include constant parameters and calculated/estimated parameters. The first ones are adopted from literature as shown in Table 5.3 while the latter are calculated for each land use and soil type within a catchment and then aggregated for each sub-catchment. The catchment parameters are calculated based on GIS/DEM processing and are assigned for each sub-catchment (Table 5.4). Since the catchment is mostly distributed by “grey soil” (Acrisols), the soil parameters are kept as unique values while other parameters are aggregated according to different land use types (Table 5.5).

Table 5.3: Constant parameters

Parameters	Notation	Units	Values
Coefficient in transport capacity relationship	A		0.00066
Power in transport capacity relationship	B		1.61
Power in the depth-discharge relationship parameter	β		1.667
Overland flow resistance	K_r		130.3
Water specific weight	γ		9.80E+03
Density of water	ρ	kg/m ³	1.00E+03
Gravity	g	m/s ²	9.80E+00
Shield sediment function	ϕ		3.76E-02
Shield criterion Reynold number	R*		4.66E+00
Kinematic viscosity of water	ν	m ² /s	1.00E-06

Table 5.4: Catchment parameters

	Slope (S_o)	Area (ha)	Overlandflow length (m)
Sub 1	0.21	266	272.80
Sub 2	0.005	811	555.2
Sub 3	0.006	389	262.4
Sub 4	0.006	621	262.4
Sub 5	0.002	87.9	60.0

Table 5.5: Soil and land use parameters

Sub-catchment	$D_{50}^{(*)}$	$\sigma^{(*)}$	$D^{(*)}$ (kg/J)	$GC^{(*)}$	$CF^{(*)}$
Sub 1	0.0001	2.10	2.00E-05	0.1 – 0.8 (0.73) ^(**)	0.35 – 0.9 (0.40)
Sub 2	0.0001	2.10	2.00E-05	0 – 0.9 (0.55)	0 – 0.9 (0.54)
Sub 3	0.0001	2.10	2.00E-05	0 – 0.9 (0.68)	0 – 0.9 (0.44)
Sub 4	0.0001	2.10	2.00E-05	0 – 0.9 (0.47)	0 – 0.9 (0.59)
Sub 5	0.0001	2.10	2.00E-05	0.1 – 0.6 (0.47)	0.5 – 0.9 (0.61)

(^{*}): Look-up table (see appendix 6)

(^{**}): Min – max (aggregated values)

5.4. Nutrient component (diffuse sources)

5.4.1. Loading functions

Simulation of nutrient transport at catchment scale is complex , especially due to its diffuse sources. Detailed description of involved processes over the whole land surface is simply impossible. One technique used to estimate the nutrient loading from land areas to receiving water is the loading function. This method has been applied in some popular models, from simple ones e.g. ANGPS (Young et al., 1995), CNS (Haith and Tubbs, 1981; Haith et al., 1984), GWLF (Haith et al., 1992) to complex ones such as CREAMS, GLEAMS (Knisel et al., 1993; Knisel and Walter, 1980), SWAT (Arnold et al., 1994), ANSWERS (Beasley et al., 1980; Bouraoui et al., 2002). Novotny and Olem (1994) considered this model alone as *screening models* to crudely estimate pollutant loads. However, it can be integrated with other interacting processes like hydrology, erosion/sedimentation. In this thesis the algorithm applied in the CNS model (Haith and Tubbs, 1981; Haith et al., 1984) is adopted. The algorithms were chosen since it is applicable for areas with limited data.

$$LD_{kt} = 0.1Cd_{kt}Q_{kt}TD_k \quad (\text{eq. 5.22})$$

$$LS_{kt} = 0.001 C_{Skt}X_{kt}TS_k \quad (\text{eq. 5.23})$$

Where:

- LD_{kt}, LS_{kt} = Dissolved and solid-phase losses of a pollutant , kg/ha
- Cd_{kt}, C_{Skt} = Pollutant concentrations in dissolved and solid-phase forms, mg/l
- Q_{kt} = Runoff, cm
- X_{kt} = Soil loss, ton/ha
- TD_k, TS_k = Transport factors which indicate the fractions of dissolved and solid-phase pollutants that move from the edge of the source area to the catchment outlet.
If dissolved pollutant are considered to be conserved, then all edge-of-field

losses will reach the catchment outlet, and the transport factor for dissolved losses is $TD_k = 1$ for all source areas

$$TSk = 2.5 d_k^{(-0.36)}$$

d_k = The down slope distance from the centre of source area k to the nearest identifiable drainage channel, m. It is assumed that dk is equal to the overlandflow length.

0.1 = The top centimetre is available for runoff loss (Haith et al., 1984)

0.001 = 1/1000 = Conversion factors for bulk density (Haith et al., 1984)

The most difficult parameters to quantify in the above equations are the pollutant concentrations in dissolved and solid-phase forms (Cd_{kt} , Cs_{kt}). While the latter can be vaguely estimated based on soil sampling before the event or from literature, the first one is trickier since it is extremely hard to collect water samples from surface during storm events. Therefore, in this thesis the chemical available for runoff (Cd_{kt}) is calculated based on the method in GLEAMS (Knisel et al., 1993) as follows:

$$C = C_1 \exp \left[\frac{-(F - ABST)}{(K_d) \left(\frac{1 - POR}{2.65} \right) + POR} \right] \quad (\text{eq. 5.24})$$

Where:

C = Chemical concentration in dissolved form (but not the final one, see eq.5.26), g/kg

C_1 = Chemical concentration or chemical mass/soil mass equal to Cs_{kt} in eq.5.22, g/kg

F = Total storm infiltration (or rainfall minus runoff), cm

POR = Porosity of surface layer

ABS = Initial abstraction from rainfall, cm

In this GLEAMS modeling approach, the abstraction is modelled continuously and relates to soil information which is not available in this study. Thus, this formula is modified as assuming the total storm runoff infiltration minus the initial abstraction (the numerator in the exponential function) is equal to the continuing abstraction (F_a), see Figure 5.6 in (Chow et al., 1988, p.147). Thus, the formula becomes:

$$C = C_1 \exp \left[\frac{-(P - Pe - Ia)}{(K_d) \left(\frac{1 - POR}{2.65} \right) + POR} \right] \quad (\text{eq. 5.25})$$

Where:

P = Total rainfall

Pe = Rainfall excess

Ia = Initial abstraction

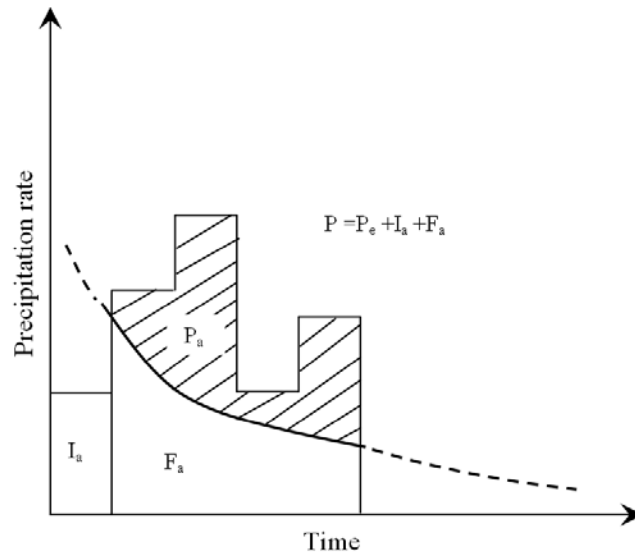


Figure 5.6: Variable in the SCS method of rainfall abstraction (Chow et al., 1988, p.147)

The final dissolved concentration is calculated based on the GLEAMS approach (Knisel et al., 1993) which is also applied in the ANSWERS model (Bouraoui et al., 2002)

$$C_s = \frac{C_{fin} \beta}{1 + k\beta} \quad (\text{eq. 5.26})$$

Where:

- C_{fin} = Equal to C in eq. 5.24
- C_s = Concentration of nutrient in solution, equal to $C_{d_{kt}}$ in eq.5.22
- β = Extraction coefficient
- k = Partition coefficient

$$\begin{cases} \beta = 0.5, & k \leq 1 \\ \beta = 0.598e^{-0.179k}, & 1 < k \leq 10 \\ \beta = 0.1, & k > 10 \end{cases}$$

Nitrate is not attached to the soil particles and is always in solution (e.g. in overlandflow, infiltrating, percolating water). In modeling nitrate, the partitioning coefficient is set to zero and the extraction coefficient is 0.5.

5.4.2. Model setup (development)

5.4.2.1. Model specialization

Data requirement for this nutrient loading model is rather simple. Hourly input data for the nutrient loading component i.e. runoff (Q_{kt}) and soil loss (X_{kt}) are obtained from the hydrology and erosion/sedimentation modules. Other parameters e.g. soil porosity, solid-phased concentration are estimated from literature or soil sampling. Model outputs are constituent loadings (hourly) at each outlet of the sub-catchments which will be later used as input for the flow routing module.

5.4.2.2. Model parameterization

The nutrient parameters are calculated for each land use type and are aggregated for each sub-catchment. Results are shown in Table 5.6. The soil porosity of 0.6 is applied for the whole catchment and is subject to calibration. The overlandflow length is similar in those applied the erosion/sedimentation module. The calibrated values of Cd_{kt} , Cs_{kt} are to that one smaller than those observed by experiment (e.g. in Kang and Lal, 1981). The reason can be due to the retention effects within the catchment as well as because of aggregation technique in GIS processing.

Table 5.6: Aggregated values of nutrient parameters

	Cd_{kt}			Cs_{kt}		TD_k	TS_k
	PO_4 (mg/l)	NH_4 (mg/l)	NO_3 (mg/l)	PO_4 (mg/l)	NH_4 (mg/l)		
Sub 1	0.0006	0.0004	0.02	0.11	0.05	1.00	0.305
Sub 2	0.0014	0.0010	0.04	0.25	0.12	1.00	0.314
Sub 3	0.0013	0.0008	0.03	0.23	0.10	1.00	0.240
Sub 4	0.0018	0.0011	0.05	0.33	0.13	1.00	0.310
Sub 5	0.0011	0.0011	0.05	0.2	0.13	1.00	0.371

5.5. River routing component

5.5.1. River network representation and assumptions

5.5.1.1. System representation

The river routing component is adapted from the D-POL model (Chu et al., 2008). The model was applied for simulating dissolved nutrients in small Mediterranean catchments during flood events. The D-POL model is an integrated system including catchment pollutant loads driven by rainfall and river routing. However, only the river routing is adopted since other model components of D-POL do not include particulate pollutants which is caused by erosion/sedimentation processes.

The most important assumption in this river routing is that *pollutant concentration is conservative* along the river reaches during storm events.

The river is discretized into reaches and each reach is discretized into a number of reservoirs depending on the length of each reach. Figure 5.7 shows how pollutant sources, sinks and changes of storages are conceptualized within reach. Figure 5.8 shows how the reaches are connected within a catchment.

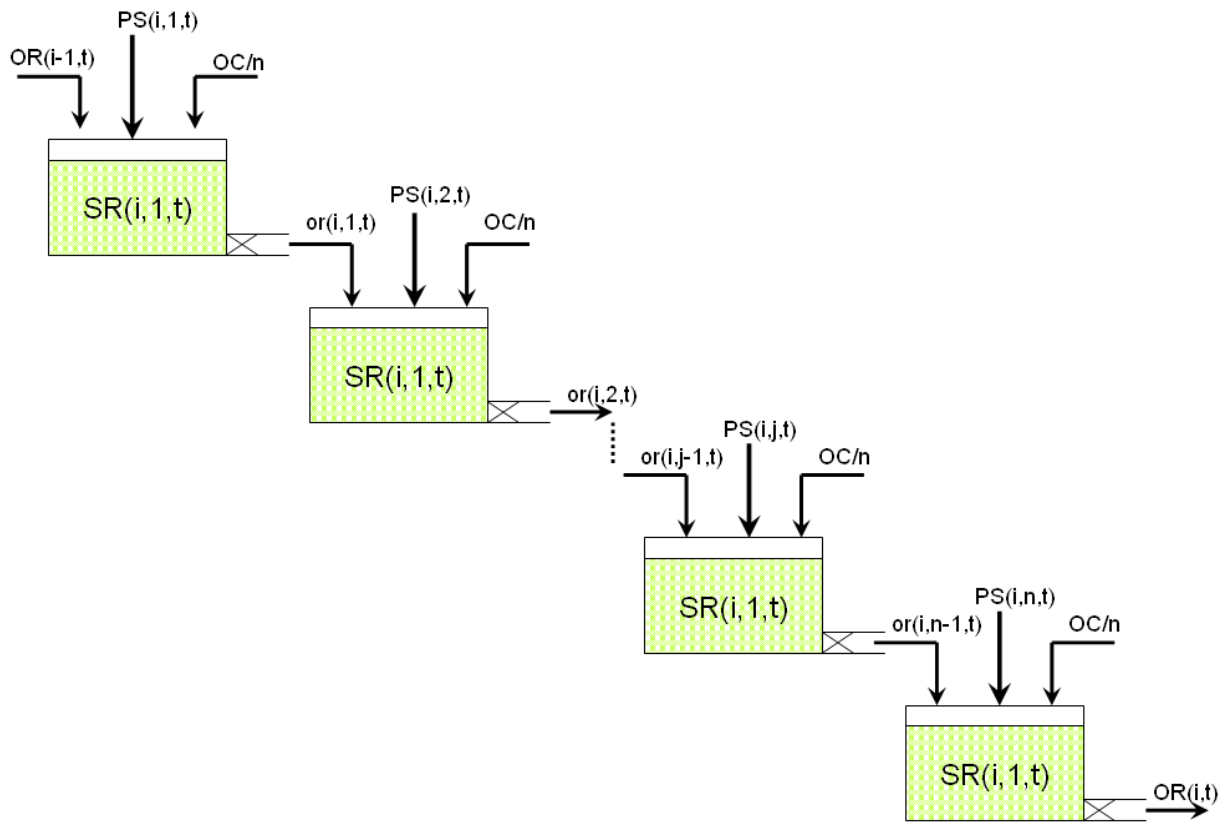


Figure 5.7: A conceptualized river reach (modified from Chu et al., 2008); see equations from eq.5.27 to eq. 5.32 for explanation of acronyms

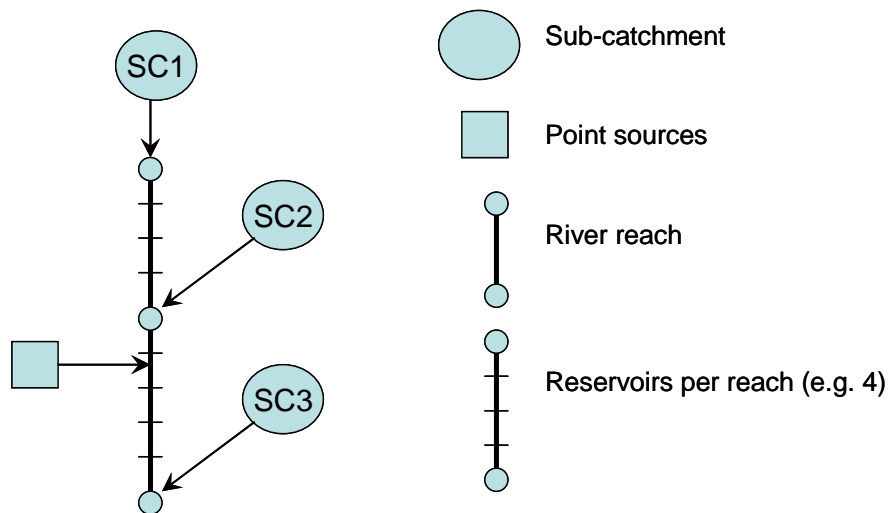


Figure 5.8: A virtual catchment (modifie from Chu et al., 2008)

5.5.1.2. Model algorithms

Equations for each reach and reservoir are based on the mass conservative principle where the change of a storage is equal to the difference between output and input. Equations referring to Figure 5.7 are as follows:

The changes of storage at reach i^{th} , 1st reservoir, time t :

$$\frac{dSR(i,1,t)}{dt} = PS(i,1,t) + \frac{OC(ci,t)}{n(i)} + OR(i-1,t) - or(i,1,t) \quad (\text{eq. 5.27})$$

The changes of storage at reach i^{th} , j^{th} reservoir, time t :

$$\frac{dSR(i,j,t)}{dt} = PS(i,j,t) + \frac{OC(ci,t)}{n(i)} + or(i,j-1,t) - or(i,j,t) \quad (\text{eq. 5.28})$$

The changes of storage at reach i^{th} , n^{th} reservoir (last reservoir of reach i), time t :

$$\frac{dSR(i,n,t)}{dt} = PS(i,n,t) + \frac{OC(ci,t)}{n(i)} + or(i,n-1,t) - OR(i,t) \quad (\text{eq. 5.29})$$

$$or(i,j,t) = \frac{1}{\tau} SR(i,j,t) \quad (\text{eq. 5.30})$$

$$T = \frac{1}{\tau} \quad (\text{eq. 5.31})$$

$$n(i) = \frac{L(i)}{Lb} \quad (\text{eq. 5.32})$$

Where:

$SR(i,j,t)$	=	Stock in the j^{th} reservoir of the i^{th} reach (kg)
$n(i)$	=	Total number of reservoirs of the i^{th} reach
$L(i)$	=	Length of the i^{th} reach
$PS(i,j,t)$	=	Point sources input (kg/h) to reservoir j^{th} of the i^{th} reach
$OC(ci,t)$	=	Pollutant input from the related c_i sub-catchment (kg/h)
$OR(i,t)$	=	Pollutant output from the i^{th} reach (kg/h)
$or(i,t)$	=	
τ	=	The lag-time of the river reservoirs (h)
Lb	=	Basic length (e.g. 1000m)
T	=	Transport parameter (1/h) (to be fitted by calibration)

5.5.1.3. Solution for the ordinary differential equations

Since the original code from D – POL is not available, solutions for the ordinary differential equations are based on the *Level Pool Routing* methods given in Chow et al. (1988). This method was adapted to the existing modeling systems. The most important assumption in this method is that the variation of inflow and outflow over the interval is approximately linear. The solution for the equation eq. 5.28 is, consequently as follows:

$$\begin{aligned} SR(i,j,t+1) - SR(i,j,t) = & (OC(i,j,t) + OC(i,j,t+1)) \times \frac{\Delta t}{2} + \left(OR(i,j-1,t) + OR(i,j-1,t+1) \right) \times \frac{\Delta t}{2} \\ & + (PS(i,j,t) + PS(i,j,t+1)) \times \frac{\Delta t}{2} - (OR(i,j,t) + OR(i,j,t+1)) \times \frac{\Delta t}{2} \end{aligned}$$

$$SR(i, j, t+1) = \left[\begin{aligned} &OC(i, j, t) + OC(i, j, t+1) + OR(i, j-1, t) \\ &+ OR(i, j-1, t+1) + PS(i, j, t) + PS(i, j, t+1) \end{aligned} \right] \times \frac{\Delta t}{2} \\ - (OR(i, j, t) + OR(i, j, t+1)) \times \frac{\Delta t}{2} + SR(i, j, t)$$

Replace $or(i, j, t) = \frac{1}{\tau} SR(i, j, t) = T \times SR(i, j, t)$

$$SR(i, j, t+1) = \left\{ \begin{aligned} &OC(i, j, t) + OC(i, j, t+1) + OR(i, j-1, t) + \\ &OR(i, j-1, t+1) + PS(i, j, t) + PS(i, j, t+1) \end{aligned} \right\} \times \frac{1}{1 + T \times \Delta t} + SR(i, j, t)(1 - T) \times \Delta t \quad (\text{eq. 5.33})$$

5.5.2. Model setup (development)

5.5.2.1. Catchment discretization

The Tra Phi catchment is discretized into 5 sub-catchments corresponding to 5 reaches. This discretization is based on the similarity (soil, topology) within a sub-catchment. In addition, each reach is discretized into a number of reservoirs depending on their lengths e.g. about 1000 meter for each reservoir (Figure 5.9, Figure 5.10 and Table 5.7)

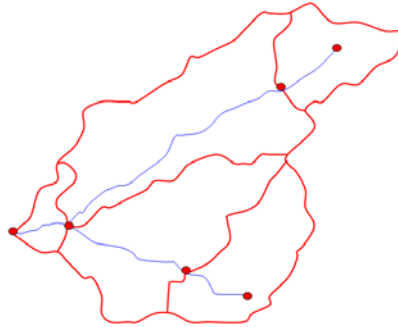


Figure 5.9: Sub-catchment delineation based on DEM processing

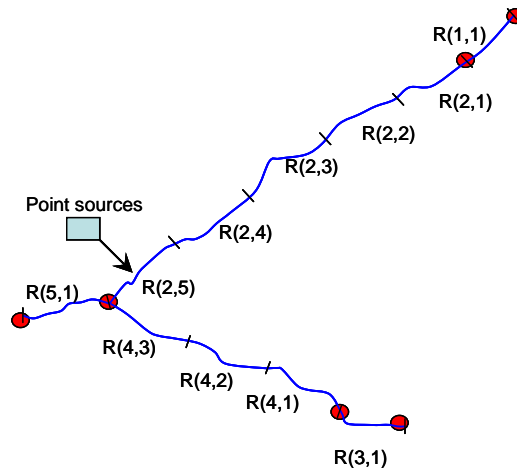


Figure 5.10: Main river network and river reach discretization (~ 1000 m each reservoir)

5.5.2.2. Model specification

The module simulates flood events on a hourly time step. Data input for this flow routing are:

- Diffuse source: sediment and nutrient loadings from sub-catchment (these are calculated the from sediment and nutrient module)
- Point source: Wastewater loadings from company at a specified location for each simulated constituents (here, from Figure 5.10 it is located at reach 2, reservoir 5)
- Reach length, average velocity (model parameters)
- Initial conditions: for each simulated constituents

Constituent loadings can be read at every reservoir, reach (as output). Concentration can only be produced at catchment outlets where flow discharge is available for converting loading to concentration.

5.5.2.3. Model parameterization

Using GIS processing, information on Tra Phi river reaches are shown in Table 5.7, Table 5.8

Table 5.7: Tra Phi reaches/reservoir information

Reach	Length (m)	Number of reservoirs	Calibrated average flow velocity - V (m/s)	Travel time per reservoir - T (hours)
1	1738	1	0.64	0.75
2	5536	5	0.48	0.64
3	1110	1	0.64	0.67
4	2639	3	0.48	0.51
5	1544	1	0.40	0.77

Table 5.8: Initial pollutant input from the sub-catchments (OC) (kg/h) (*)

Sub-catchment	TSS	P-PO ₄	N-NH ₄	N-NO ₃
Sub 1	72	0.054	0.036	0.108
Sub 2	216	0.162	0.108	0.324
Sub 3	72	0.054	0.036	0.108
Sub 4	360	0.27	0.18	0.54
Sub 5	1969	1.24	0.39	1.44

(*) reference: field observation

5.6. Simulation results

5.6.1. Sensitivity analysis

Model parameters are analyzed for 4 main model modules (i.e. hydrology, erosion, nutrient loading, and river routing). Table 5.9 shows the parameters and their variations applied in this analysis. The sensitivity is calculated based on perturbing the model parameters within the ranges and observing the variation of model results (e.g. total flow discharge or total loadings for the whole event). An example

resulting from the sensitivity analysis for nutrients is shown in Figure 5.11, others are presented in appendix 5. It can be concluded as follows:

- Within the hydrological components, the CN value and the rainfall input are the most sensitive factors to model results. The CN value is more sensitive than the rainfall input to the variation of flow discharge volume. The velocity parameters (Vo, Vs) do not change the total volume but only influence the shape of hydrograph.
- The parameters/inputs from the hydrology parts are most sensitive to sediment and nutrient generation processes. The CN values and rainfall are still the most sensitive ones. The velocity parameters (V from river routing module and Vo, Vs from hydrological module) are the next sensitive parameters. The effects from the velocity to the shape of hydrograph will significantly contribute to total loadings since the loading is a function of flow discharge and concentration.
- The effects of soil parameters(D (K), D₅₀, POR) is very small to the final results of sediment and nutrient loadings if compared to hydrological parameters. In addition, the nutrient loading parameters (i.e. Cdk (N-NO₃), Csk (P-PO₄, N-NH₄)) can only show clear variations when increasing up to 500%.
- The changes of point sources also affect considerably the model results. The variation is about 35% when the perturbation is less than 50%. However, when increasing the perturbation to 5 times (500%), the variation is about 280%. This aspect is essential when dealing with illegal wastewater disposal as discussed in chapter 4.

From these results, **a key message** for simulating the coupled system is that the calibration of hydrological part should be carefully performed before applying other model components.

Table 5.9: Model parameters used for sensitivity analysis

Acronyms	Description	Range
Hydrology		
CN	Curve Number	± 20%
Rain	Rainfall (mm)	± 20%
Vo	Overlandflow velocity (GIUH module)	± 20%
Vs	Average stream velocity (GIUH module)	± 20%
Erosion		
D (K)	Soil erodibility factor	± 20%
D50	Median size of soil particle	± 20%
POR	Porosity of surface soil layer	± 20%
Nutrient loading		
Cdk (N-NO ₃)	N-NO ₃ concentrations in dissolved forms	± 500%
Csk (P-PO ₄)	P-PO ₄ concentrations in solid-phase forms	± 500%
Csk (N-NH ₄)	N-NH ₄ concentrations in solid-phase forms	± 500%
River routing		
V	River reach velocity (Flow routing module)	± 20%
Point sources		
TSS	TSS point sources (hourly)	± 500%
P-PO ₄	P-PO ₄ point sources (hourly)	± 500%
N-NH ₄	N-NH ₄ point sources (hourly)	± 500%
N-NO ₃	N-NO ₃ point sources (hourly)	± 500%

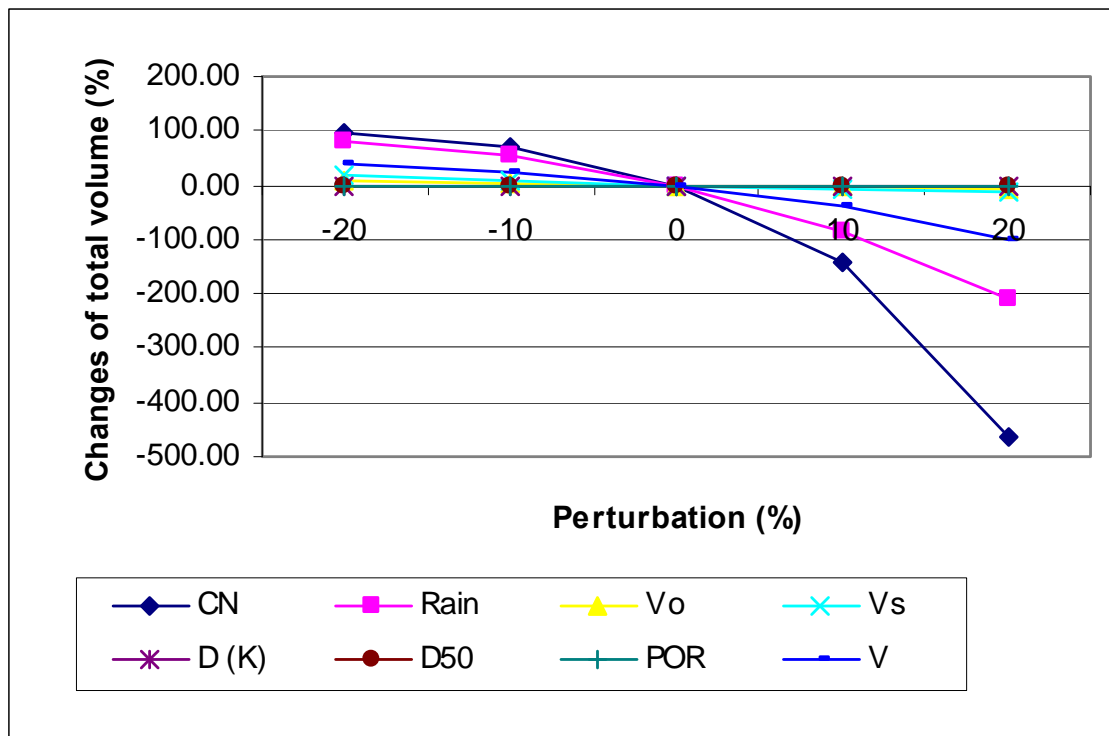


Figure 5.11: Sensitivity analysis for nutrients (hydrological and soil erosion parameters)

5.6.2. Model results

The hydrological parameters and inputs (e.g. CN, rainfall) significantly affect the results of other results (sediments, nutrients). So, these parameters need carefully be calibrated before considering other parameters.

Table 5.10 shows evaluation parameters for flow, TSS, P-PO₄, N-NH₄, N-NO₃. The parameters are also illustrated in Figures (Figure 5.12 to Figure 5.16). It can be concluded as follows:

- The surface flow discharge is well simulated including the curve, peak, and time to peak. A good agreement is also given between simulated sediment, nutrient and observed values, especially at the raising curve and peaks.
- According to Table 5.10, based on the PBIAS parameter, the simulated hydrograph fits well to the observed hydrograph. In addition, the sediment simulation as well as the nutrients simulation is also satisfactory (within the range). Furthermore, the d index shows a good agreement between simulated and observed variables (flow discharge, sediments and nitrate nitrogen); however, it is not very good for ammonium and phosphate.
- Prediction of nitrate nitrogen (N-NO₃) is better comparing to ammonium (N-NH₄) and phosphate (P-PO₄). The reason could be that is related only to runoff processes, while the other two matters depend on erosion and sedimentation processes.
- The measurement error is rather high comparing to the variation. It should be further improved by implementing more certain monitoring techniques, and a higher frequency of measurement

- The model can not capture the receding curve. As similar to the results from the HSPF model, it could be the retention effects of agricultural field, especially rice fields which were controlled by farmers (e.g. releasing water after rainfall events to ensure the field is not too much inundated)

Table 5.10: Model evaluation parameters for simulations from 25 to 27th July 2008.

	PBIAS	d	R ² (1:1)	RMSE	NSE	RSR
Flow	0.129	0.996	0.983	0.356	0.983	0.132
TSS	50.302	0.846	0.252	283.547	0.252	0.865
P-PO ₄	26.856	0.547	-0.070	0.350	-0.070	1.034
N-NH ₄	-8.299	0.593	0.178	0.242	0.178	0.907
N-NO ₃	22.436	0.831	0.412	0.467	0.412	0.767

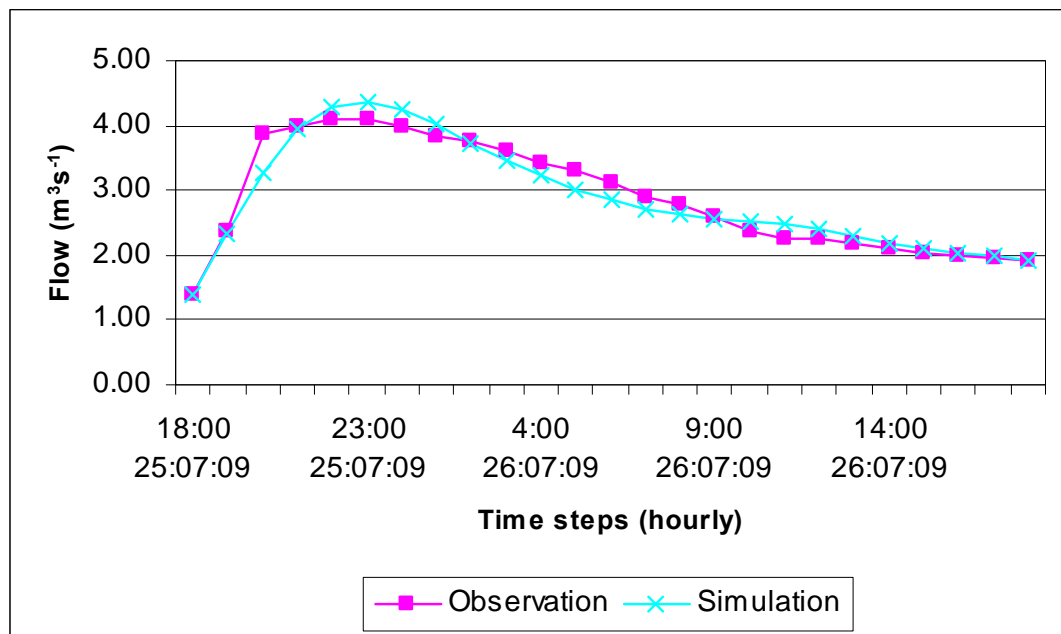


Figure 5.12: Observed and simulated flow discharge (including baseflow and interflow)

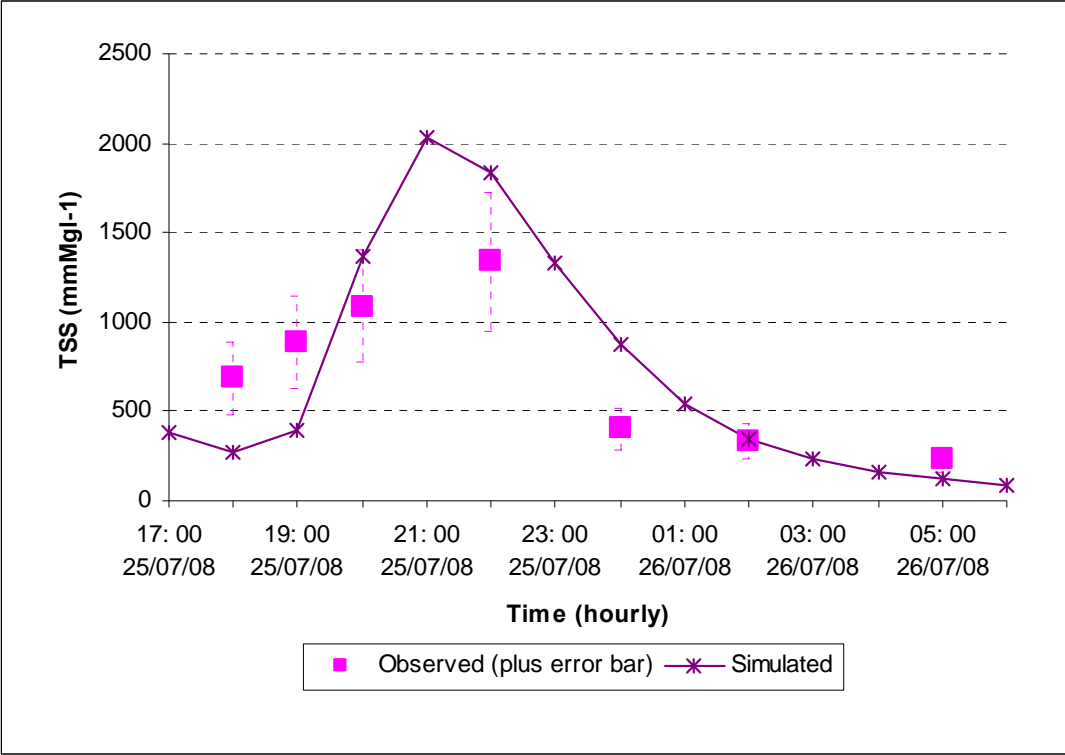


Figure 5.13: Observed and simulated suspended solid

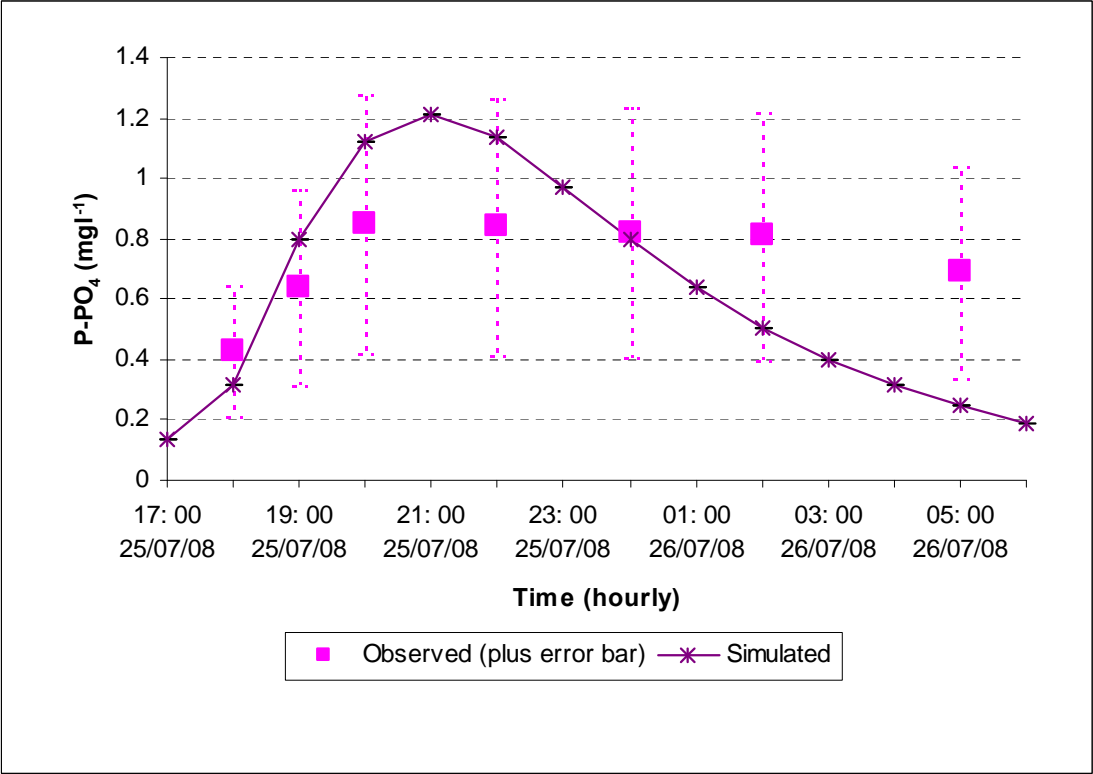


Figure 5.14: Observed and simulated P-PO₄

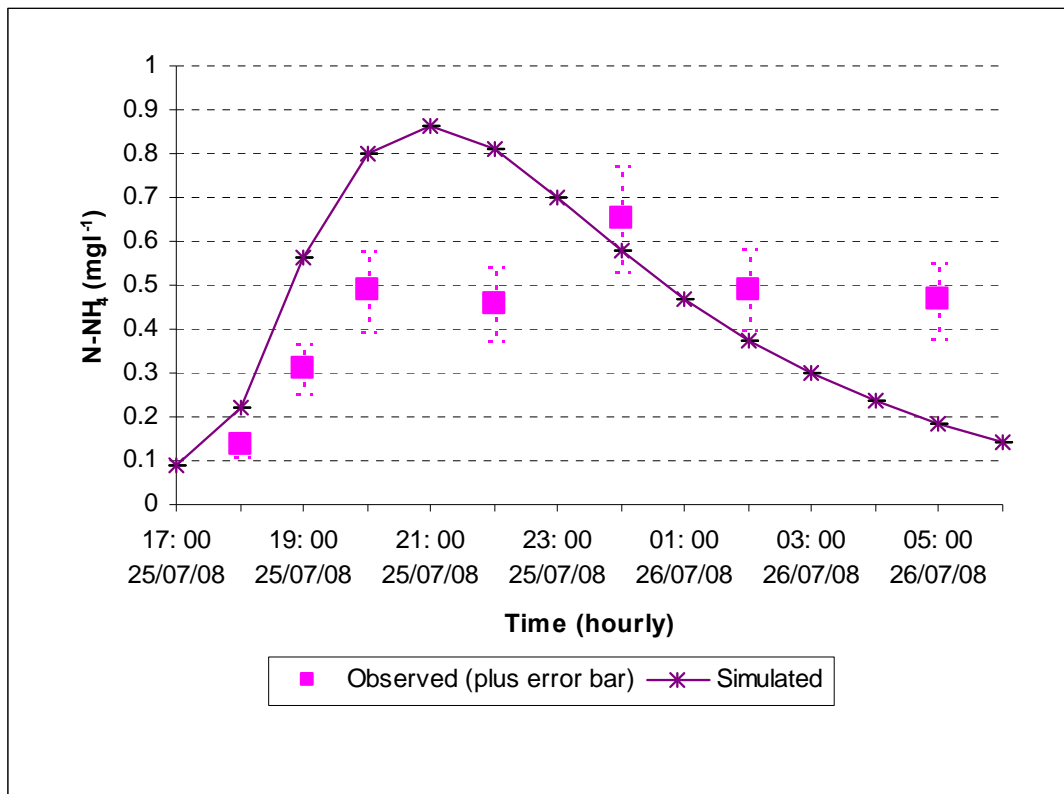


Figure 5.15: Observed and simulated N-NH_4

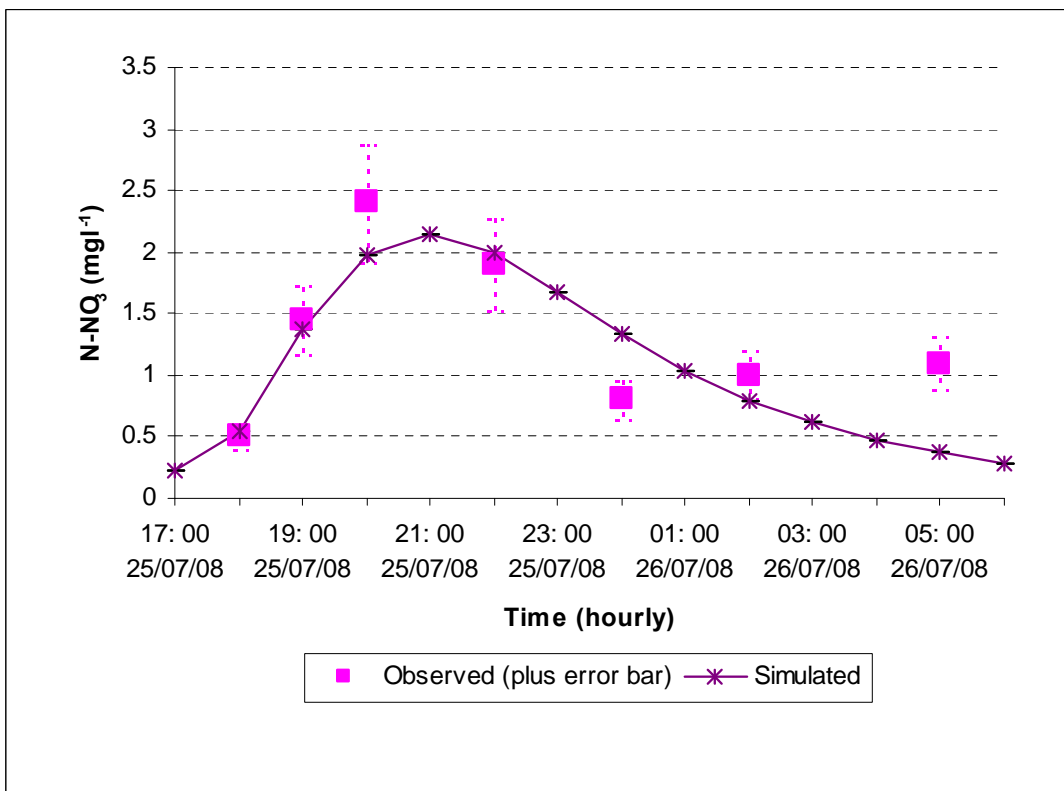


Figure 5.16: Observed and simulated N-NO_3

5.6.3. Model uncertainty

The Monte- Carlo simulation method was utilized for an uncertainty analysis. This method has been presented in section 2.6.4.2. In this thesis, the Monte Carlo simulation is combined with the Latin Hypercube Sampling method. Every simulation is run for 1000 time steps within a Microsoft Excel file. The software is assisted by an add-in programme called RiskAMP (The RiskAMP Monte Carlo Add-in for Excel®). For each parameter and input the uniform distribution is applied. Data for the Monte-Carlo simulation are shown in Table 5.11.

Table 5.11: Variation (min – max of 90% confidence) of constituents at different scenarios

Acronyms	Description	pdf	Calibrated values	(min;max)
Hydrology				
CN	Curve Number	uniform	54	(52;56)
Rain	Rainfall (mm)	uniform	40.5	(38;42)
Vo	Overlandflow velocity (GIUH module)	uniform	0.04	(0.03;0.05)
Vs	Average stream velocity (GIUH module)	uniform	0.75	(0.65;0.8)
Erosion				
D (K)	Soil erodibility factor	uniform	0.14	(0.1;0.18)
D50	Median size of soil particle	uniform	0.11	(0.05;0.15)
POR	Porosity of surface soil layer	uniform	0.6	(0.5;0.7)
River routing				
V	River reach velocity (Flow routing module)	uniform	0.8	(0.75;0.85)
Nutrient loading				
TSS	TSS point sources (hourly)	uniform	50	(30;100)
P-PO ₄	P-PO ₄ point sources (hourly)	uniform	0.8	(0.5;1)
N-NH ₄	N-NH ₄ point sources (hourly)	uniform	0.6	(0.4;1)
N-NO ₃	N-NO ₃ point sources (hourly)	uniform	1.2	(0.6;1.5)

(*): multiply factor for each land use

The sensitivity analysis showed that the CN, flow velocity (river routing) parameters and rainfall (input) are the most sensitive ones for the model results. Thus, firstly, these three parameters and the input are simulated so that the Nash_Sutcliffe efficiency (NSE) ranges within 0.85 – 0.95 which is considered as acceptable (e.g. in US EPA, 2009). Since then, different scenarios have been developed in order to see how these parameters propagate to model results. Results are shown in Table 5.12 and partly in Figures (Figure 5.17 to Figure 5.19). Other results are placed in appendix 5.

Due to the high effects of the CN parameter, rainfall and flow velocity, the propagation of other parameters is not clearly seen (Table 5.12). The uncertainty boundary is much reduced if these parameters are excluded in the uncertainty analysis. The results are also consistent with those obtained from the sensitivity analysis part.

The uncertain boundary is rather large, especially during the peak flows by comparing to the mean values it can be more than 100 percent. However, the simulation results show that when including the boundary (confidence interval of 90%) of Monte-Carlo simulation a very good agreement between model simulation and observation data is obtained.

The variation of model output is also highly effected by the change of point sources, especially when extreme disposal occurs. This was also shown in section “sensitivity analysis”, the increase of point source with about 5 times than normal can change the results up to 280%.

Table 5.12: Variation (min – max of 90% confidence) of constituents at different scenarios

Scenarios	Flow NSE	TSS peak Mg/L	P-PO ₄ peak Mg/L	N-NH ₄ peak Mg/L	N-NO ₃ peak Mg/L
1 CN	0.85 – 0.95	1600 – 3450	1 – 2.3	0.72 – 1.6	1.8 – 4.1
2 CN, rainfall	0.85 – 0.95	700 – 3000	0.8 – 2.1	0.35 – 1.22	0.8 – 3
3 CN rainfall, Vo	0.85 – 0.95	1250 – 2820	0.78 – 1.62	0.55 – 1.2	0.12 – 2.95
4 CN rainfall, Vo, Vs	0.85 – 0.95	1450 – 3100	0.9 – 1.91	0.67 – 1.39	1.82 – 3.54
5 CN rainfall, Vo, Vs, D(K)	0.85 – 0.95	750 – 2500	0.68 – 1.72	0.63 – 1.37	1.74 – 3.44
6 CN rainfall, Vo, Vs, D(K), D50	0.85 – 0.95	1550 – 32650	0.92 – 1.87	0.82 – 1.56	2.15 – 3.86
7 CN rainfall, Vo, Vs, D(K), D50, POR	0.85 – 0.95	1160 – 2840	0.37 – 1.31	0.67 – 1.39	1.05 – 2.76
8 CN rainfall, Vo, Vs, D(K), D50, POR, Cdk (NO ₃), Cskt (P-PO ₄), Cskt (N-NH ₄)	0.85 – 0.95	810 – 2650	0.81 – 2.25	0.45 – 1.37	1.85 – 4.85
9 CN rainfall, Vo, Vs, D(K), D50, POR, Cdk (N-NO ₃), Cskt (P-PO ₄), Cskt (N-NH ₄), V	0.85 – 0.95	600 – 2530	0.85 – 2.12	0.41 – 1.25	1.23 – 2.51
10 CN rainfall, Vo, Vs, D(K), D50, POR, Cdk (N-NO ₃), Cskt (P-PO ₄), Cskt (N-NH ₄), V, point sources (TSS, P-PO ₄ , N-NH ₄ , N-NO ₃)	0.85 – 0.95	1400 – 2500	1.1 – 1.8	0.42 – 1.2	1.15 – 2.8

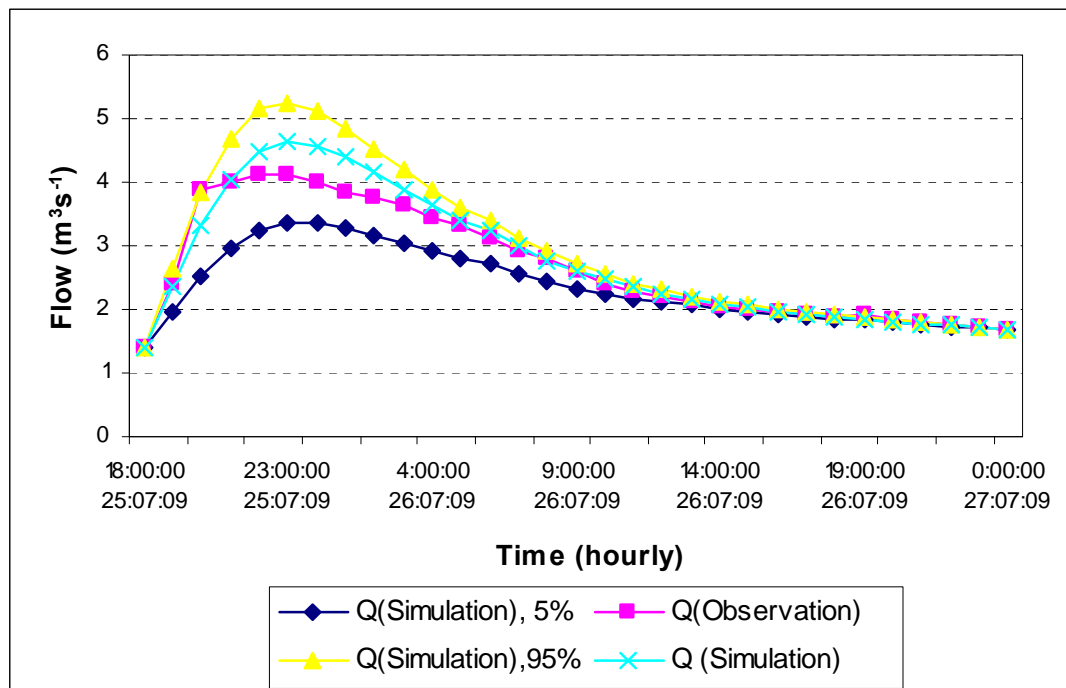


Figure 5.17: Flow simulation results (NSE:0.85 – 0.95)

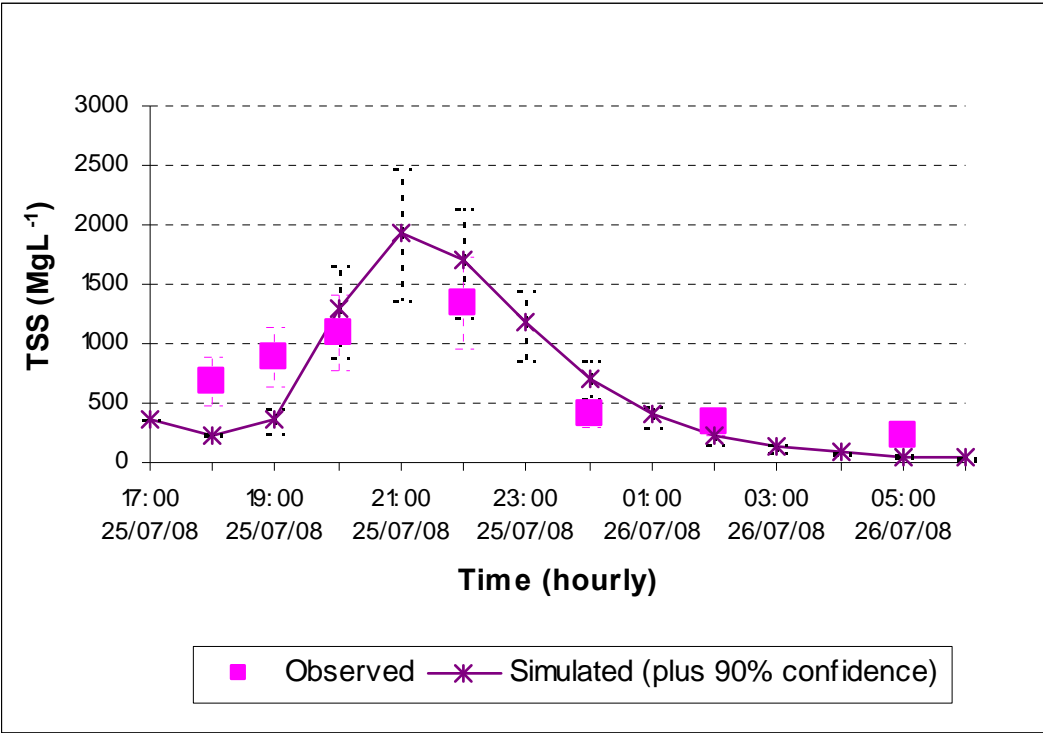


Figure 5.18: TSS simulation results

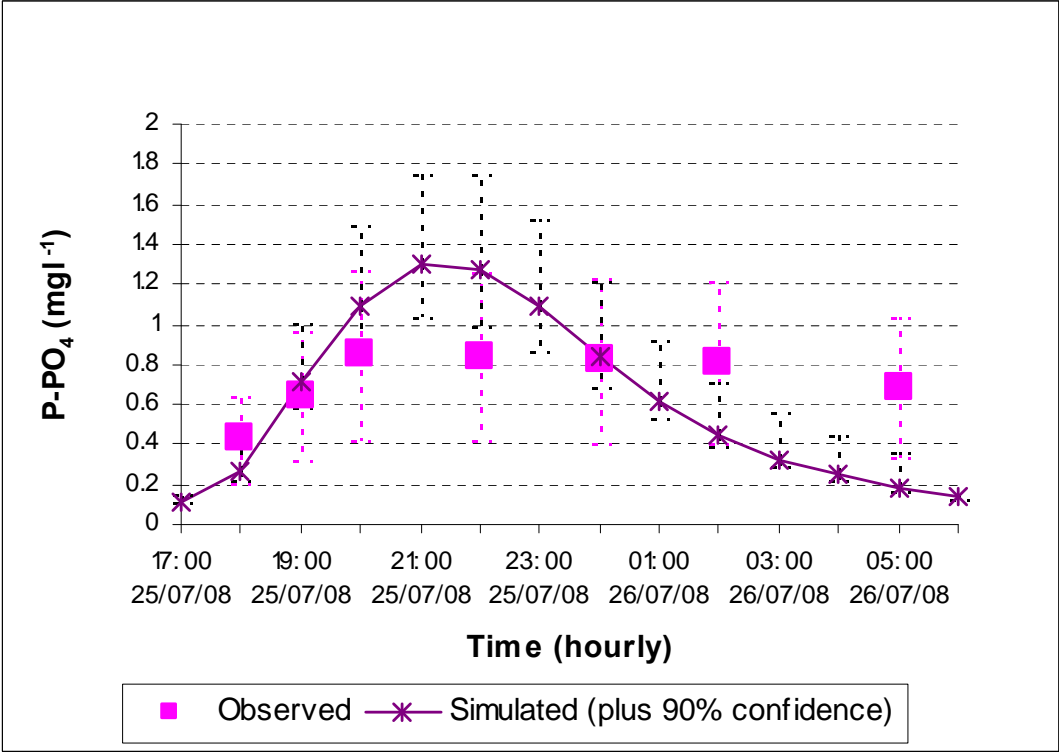


Figure 5.19: Phosphorus phosphate (P-PO₄) simulation results

5.7. Conclusion and recommendations

In this chapter, it is shown that the SINUDYM model has been developed to meet the specific demands of tropical regions. It was successfully applied for a case study in Vietnam. The conclusions are as follows:

- Simplified model structure and limited model parameters are the most appealing features of the model. All model components are coupled and controlled within one file. Affects of different model components can be easily assessed and monitored. This aspect is especially useful when implementing the sensitivity and uncertainty analysis. The coupled system can represent the system dynamics e.g. flow discharge, suspended solid and nutrients during flood events. In addition the point sources disposal is also included. The running environment is within an Excel spreadsheet, a routine package for every professional. This aspect makes the model user-friendly and robust and supports the installment of the model as operational tool for the region. Furthermore, an add-in Monte – Carlo simulation tool is tested within this modeling system providing a good uncertainty analysis tool for the users. In addition, because of the capacity of the model in utilizing GIS, remotely sensed data, many model parameters can be extracted easily. This aspect is very important when dealing with limited data areas (ungauged catchment).
- The success of the developed model has proven the importance of selecting suitable model structures. Here the GIUH, the simplified process erosion and sedimentation, the loading function and the river routing have been chosen from different existing modeling systems and been linked together. These model components have been successfully tested for tropical or extreme rainfall conditions. It is also confirmed in some publications (e.g. Kundzewicz, 2007a; Savenije, 2009), that first of all the dominant processes in the system should be captured in the model, whereas processes of minor importances should be neglected or treated in a less complex manner.
- For diffuse pollution analysis at small catchment scale, a proper simulation of the basic hydrological processes (i.e. the relation between rainfall and runoff) is the most important task. Thus this aspect has to be carefully considered before working with erosion/sedimentation and nutrient components.
- Based on the uncertainty simulation results, possible scenarios can be explored when dealing with many uncertain sources (similar conclusion in Brugnach and Pahl-Wostl, 2008). The next objective should be given to reducing the uncertainty caused by input data e.g. obtaining more reliable data by improving monitoring data in time and space. For example, the high impact to model results is also found in rainfall data. Given only one observation station in the catchment covering an area of extremely topographic variation, the uncertainty propagation due to incorrect rainfall data is a critical issue. Therefore, improving rainfall observation is a “must”.
- It is observed that the simple SINUDYM model is comparable to the complex one when applied for nutrient dynamics during flood events. For a single event simulation, the SINUDYM provides better results as the HSPF model. Figure 5.20 shows an example for the P-PO₄ simulation. In the present version, SINUDYM does not yet consider groundwater flow, which is essential for long term simulation as the HSPF does. Thus, this relative comparison

is just to confirm that, in many cases, it is possible to apply a simple model in stead of comprehensive ones.

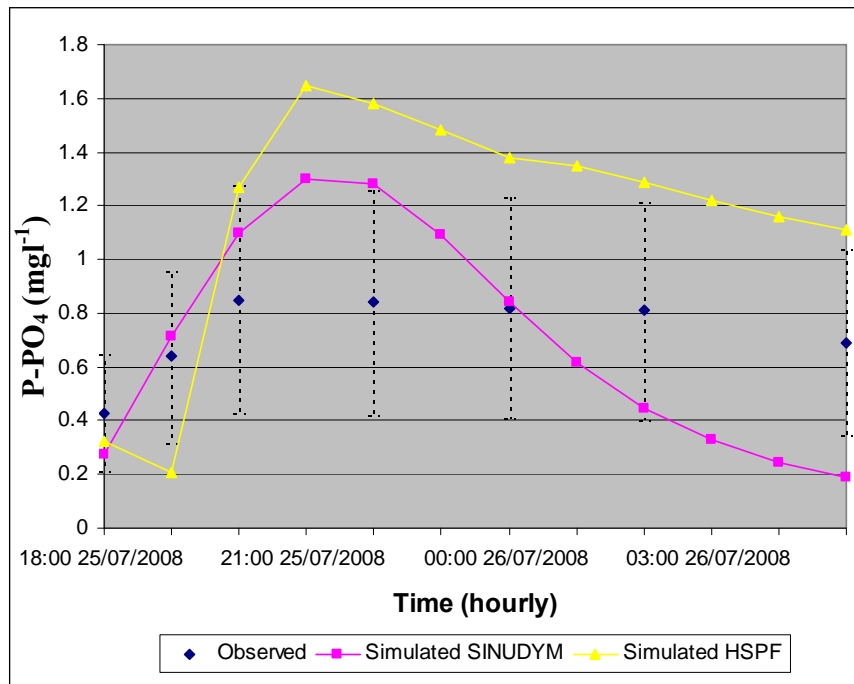


Figure 5.20: Model comparison between SINUDYM and HSPF (P-PO₄)

Several **limitations** of the model should be pointed out. These should be considered for improvements in the future. They are:

- The model is an event-based model and presently only simulates the surface runoff including intermediate flow. Groundwater flow is ignored. Therefore, it is required to either subtract groundwater from observed data, or add groundwater to the simulated data for evaluating model performance realistically (see also in Yagow, 1997)
- The SCS – Curve Number method is based on empirical equations and highly affects the simulation results. Its errors can significantly propagate through the coupled system. In addition, the CN method was developed in some regions outside Vietnam (i.e. United States of America). Therefore, further investigations on using this approach for tropical regions are required.
- In this thesis, the uncertainty due to GIS data, as well as GIS processing errors are not mentioned. This is partly because the focus is given to the development of the model processes. Therefore, for future application, accuracy assessment of GIS data must be considered.
- The model is semi-distributed; however, most of model parameters are lumped (by means of aggregating). Consequently, the model can not accurately represent the effect of different land uses, especially rice fields. Thus, this aspect should be considered for improvement so that the influence of e.g. urbanization, best management practice can be analysed.

- The assumption of transport of conservative contaminants by the flows should not be fully accepted. This assumption is based on the characteristics of high flow occurrence. During small storm and low flow conditions, this assumption is not valid. For further improvement, the incorporation of other water quality processes (e.g. described in section 4, chapter 2) can be considered.
- Since the model is programmed within an Excel spreadsheet, several operation steps have to be done manually (e.g. sub-catchment parameters, river reach discretization). For improving this aspect, an interaction with some GIS package is recommended.

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We believe conceptualising these processes requires a 'top-down' strategy of model development, i.e. keeping the model as simple (parametrically parsimonious) as possible but as complex as necessary to describe the available data well while ensuring physical and chemical relevance. Such a model would describe the dominant modes of behaviour of phosphorus transfer, where these can be supported by field observations. (Krueger et al., 2007)

6. A model-based framework for water quality management: An implication for Vietnam condition

6.1. Water quality management in Vietnam

6.1.1. Introduction

In Vietnam, together with economic development in the recent decades, environmental problems, especially water quality pollution, are being often reported in media. In the report of “The state of water environment in 3 river basins of Cau, Nhue-Day, Dong Nai river system” (VEPA, 2005), it was pointed out that the water resources in Vietnam are being degraded in both in water quality and water quantity. Extremely polluted water caused by illegal wastewater disposal as well as accidents of wastewater facilities are still observed (VEA, 2008;2009).

The Vietnamese government has paid a lot of attention for water resources management. For example, developing water-related laws, regulations, re-organizing water-related institutions, setting up more water monitoring network - are some of the significant contributions. However, successful stories are still very limited, even in some areas the problems had worsened.

In this section, firstly, a review on recent efforts from the management aspects (e.g. legal and regulatory instruments, institutional framework, monitoring network) is presented. It is followed by identifying the missing components in water quality management in Vietnam. Based on this, a framework considering catchment water quality modeling is proposed.

6.1.2. Legal and regulatory instruments

Regarding water quality management in Vietnam, legislative documents are developed surrounding the Law of Environmental Protection (1993, amended in 2005) and The Law of Water Resources (1998, amendment). A summary of the laws as well as guiding documents, decisions, directives and circulars has been reported in recent years e.g. Global Water Partnership (2003), Nguyen (2009), Truong (2007).

The important documents include:

- Decree No. 175/CP dated October 18, 1994 of the Government guiding the implementation of the Environmental law and Decree No. 143/2004/ND-CP dated July 12, 2004 on the amendment and supplement of the article 14 of the Decree No. 175/CP
- Directive No. 200/TTg dated April 29, 1994 of Prime Minister on Ensuring Clean Water and Rural Environmental Sanitation
- Decree No. 179/1999/ND-CP dated December 30, 1999 of the Government stipulating the implementation of the law on water resources

- Decree No. 162/2003/ND-CP dated December 19, 2003 of the Government stipulating the collection, management and use of data/information on water resources
- Decree No. 67/2003/ND-CP dated June 13, 2003 of the Government on the environmental fees for waste water
- Inter-ministerial Circular No. 125/2003/TTLT-BTC-BTNMT dated December 18, 2003 of the Ministry of Finance and MONRE guiding the implementation of the Decree No. 67/2003/ND-CP
- Decree No. 149/2004/ND-CP dated July 27, 2004 of the Government on regulation on licensing of water resources exploitation, extraction and utilisation and waste water discharge in water sources
- Decree No. 149/2004/ND-CP dated July 27, 2004 of the Government on regulation of water resources exploitation, extraction and utilization and waste water discharges into water resources
- Decree No. 121/2004/ND-CP dated May 12, 2004 of the Government stipulating the treatment of administrative violence in the field of environmental protection
- Decree No. 34/2005/ND-CP dated March 17, 2005 of the Government on sanctions against violations of water resources management regulations
- Decree No. 137/2005/ND-CP dated November 09, 2005 of the Government on the environmental fees for mining activity
- Circular No.:02./2005/TT-BTNMT date 24 June, 2005 of the Minister of MONRE guiding implementation of the government decree 149/2004/ND-CP regulating the licensing of water resources exploration, exploitation, utilization and waste water discharge into water sources
- Decree No. 81/2006/ND-CP dated August 09, 2006 of the Government on stipulating fining levels of administrative violations
- Decree No. 80/2006/ND-CP dated August 9, 2006 of the Government regulating in detailed and guiding the implementation of some articles of the Environmental Law on environmental standards, Environment Impact Assessment (EIA), strategic EIA, commitment on environmental protection, environmental protection in manufacturing, trade and services, hazardous waste management and publicity of data information on environment
- Decree No. 59/2007/ND-CP dated April 09, 2007 of the Government on solid waste management
- Decree No. 120/2008/ND-CP dated December 1, 2008 of the government on River Basin Management
- Decree No. 112/2008/ND-CP dated October 20, 2008 of the government on management, protection and integrated utilization of natural resources and environment at irrigation and hydro-electric reservoirs
- Circular No.:02./2009/TT-BTNMT dated March 19, 2009 of the Minister of MONRE regulating assessment of receiving wastewater capacity of water resources

In the Law of Environmental Protection, chapter 7 focusing on water quality management, in which, the most important aspects are:

- Responsibility of local governments in the river basin to ensure benefits of utilizing water for the whole community
- Activities concerning water pollution in the river basins have to be reported at relevant level (local or central government) on “Environmental Status” and “Environmental Impact Assessment” (e.g. pollution sources, discharge conditions, development of new production, business and service areas, urban areas and populated residential areas in the river basins)
- Cooperation among provinces where river crossing (e.g. through River Basin Organization)
- Wastewater management (collection, treatment, building of treatment systems)
- Pollution remediation and environment restoration

The Law of Water Resources stipulates the general regulations on water resources management, protection, exploitation and utilization; as well as prevention and remediation of damage and negative impacts caused by water. Concerning the protection of water quality, the Law requires that there must be a plan to prevent and control water pollution and restore the quality of the polluted water source; Activities relating water resources should be harmonized with the Law of Environmental Protection. It is strictly prohibited to introduce into the water sources any noxious water, untreated wastewater or wastewater that has been treated but still does not meet the permissible standards (*Nguyen, 2009*).

One of the most important bases for regulating water quality management is water quality standards. The standards stipulate the allowable limits for the ambient water quality parameters and the contents of pollutants in ambient water and waste water. The standards, most related to the water quality in river basins are:

- TCVN 5945-2005: requirements for discharged industrial water
- TCVN 5942-1995: requirements for ambient surface water quality standard
- TCVN 5943-1995: requirements for coastal water quality standard
- TCVN 5944-1995: requirements for groundwater water quality standard
- TCVN 6773:2000: water quality guidelines for irrigation
- TCVN 6774-2000: water quality guidelines for protection of aquatic life

In addition, there are also 2 important national strategies:

- National Strategy on Water Resources to 2020 No.81/2006/QĐ-TTg signed by the Prime Minister on 14/04/2006
- National Strategy for Environmental Protection until 2010 with vision toward 2020 signed by Prime Minister on 02/12/2003

These stipulate focus on:

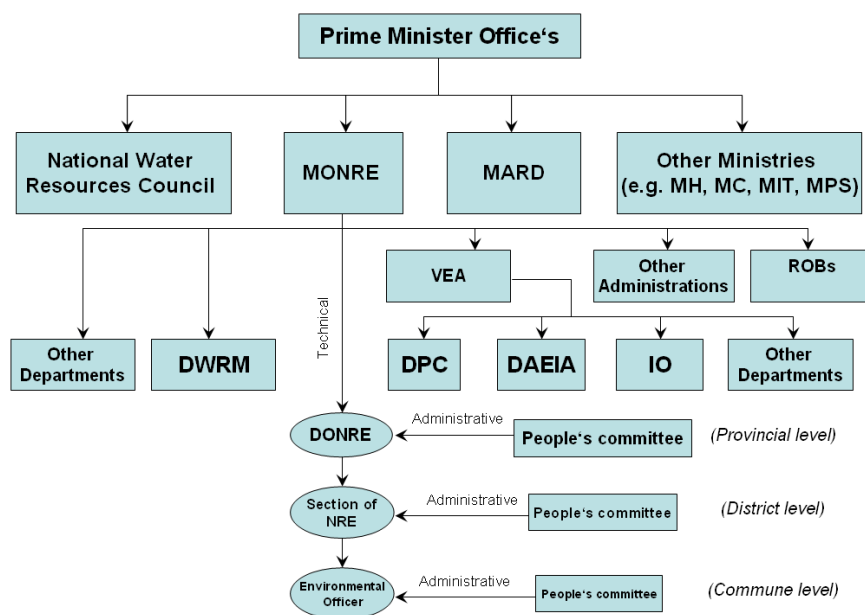
- Development of institutional arrangements and capacity building for water resources management in accordance with the integrated management approach at the basin scale
- Support to provinces in technology, methodology and equipment for water quality monitoring.

- Education and training for public awareness rising on the water resources protection and management and development of the relevant national information system
- Development of international cooperation with focus on bilateral cooperation in the fields of environment, water resources for the provinces. Strengthen the cooperation between the provinces of Vietnam
- Development of organizational mechanism and operation modality of the multi-stakeholder water resource related committees, such as River basin committee
- Development of transparent and efficient financing mechanism

It is observed that although many aspects have been regulated in the legal and regulatory documents. However, the regulations are still in a very general form, detailed instructions are very limited regarding for implementation at local and regional levels. In addition, lacking of human resources including expertise is also others constrains in water quality management. These aspects will be further analysed in the following sections.

6.1.3. Institutional framework

Figure 6.1 provides an institutional frame for local, central government relating to water resources management in Vietnam. Functional descriptions of these institutions are presented in the following.



VEA: Vietnam Environment Administration
DWRM: Department of Water Resources management
DPC: Department of Pollution Control
DAEIA: Department of Appraisal and Environmental Impact Assessment
IO: Inspection Office
DONRE: Department of Natural Resources and Environment
NRE: Natural Resources and Environment

MONRE: Ministry of Natural Resources and Environment
MARD: Ministry of Agriculture and Rural Development
MH: Ministry of Health
MIT: Ministry of Industry and Trade
MC: Ministry of Construction
MPS: Ministry of Public Security
RBO: River Basin Organization

Figure 6.1: Main organizational arrangement related to water quality management (partly selected from Hansen and Do, 2005; Truong, 2007)

The Ministry of Natural Resources and Environment (MONRE) is responsible for water resources and environmental management. Relating water quality management, the MONRE have to work on, for example, water resources planning, implementing strategy, appraisal & assessment of environmental-affected projects, preventing water degradation (quantity and quality), controlling and restoring water pollution, issuing environmental standard, monitoring. The Ministry also solves cross-sectoral and inter-provincial problems (e.g. river basin planning). Main assistants to the MONRE are the Vietnam Environment Administration (VEA) and Department of Water Resources management (DWRM). The VEA focuses on environmental problems (i.e. water pollutions), whereas, DWRM works on water quantity issues (e.g. water balance, water resources assessment). Department of Pollution Control (DPC), Department of Appraisal and Environmental Impact Assessment (DAEIA) are the two important offices supporting VEA for water quality management in reviewing, assessing environmental plan from companies, industrial zones. In addition, Inspection Office (IO) of VEA is mobilized if there is any suing or accidental problem occurs.

Detailed descriptions on functions and responsibilities of MONRE, VEA, and DWRM are listed in a number of documents, for example:

- Decree No. 25/2008/ND-CP dated March 04, 2008 of the government stipulating functions, tasks, authorities, and organizational structure of the Ministry of Natural Resources and Environment
- Decision No. 132/2008/QĐ-TTg September 30, 2008 of the Prime Minister stipulating functions, tasks, authorities, and organizational structure of the Vietnam Environment Administration (VEA) of the Ministry of Natural Resources and Environment
- Decision No. 1035/QĐ-BNTMT dated May 19, 2008 of the Minister of MONRE stipulating functions, tasks, authorities, and organizational structure of the Department of Water Resources Management (DWRM) of the Ministry of Natural Resources and Environment

Another Ministry most concerned about water resources management is the Ministry of Agriculture and Rural Development (MARD). In this Ministry, activities such as management of flood and typhoon protection system, hydraulic structure, wetland management, rural water supply and sanitation usually interact very much with those activities carried by MONRE. For example, the MONRE has to keep minimum water flow (for ecosystem preservation), while the MARD has to provide enough water for agriculture activities or subsidizing water use. Management of fertilizer used in agriculture or food for aquaculture activities relating very much on water quality are also under MARD. It should be noted that the DWRM once belonged to MARD. The re-organization just took place few years ago.

Other Ministries like Ministry of Health (MH) has responsibility in ensuring drinking water quality; Ministry of Industry and Trade (MIT) develops Hydro power construction; Ministry of Construction (MC) is responsible for building urban water supply, sanitation, and drainage facilities. Due to the complexity of managing illegal waste, wastewater pollution disposal, on 29/11/2006, the Minister of Ministry of Public Security (MPS) of Vietnam established Department of Environment Security. Since then the violence of environment (including water resources) can also be regulated in “Criminal Law”.

There are not always projects carrying out by one Ministry affecting positively to other ministries. Therefore, in addition to MONRE, the National Water Resources Council consults for the government on important water issues. They are: national policy, strategy, large river basin planning, water transfer

among big rivers, water national hazards, solution for conflicts among ministries and central provinces.

Establishing the River Basin Organizations (RBOs) is a recent effort from the government to effectively manage river basins crossing provinces. The RBOs is responsible for investigating environmental base of water resources, river basin planning, protecting, allocating water resources, river basin management, etc. they also propose solutions, policy concerning water resources protection and use for the whole river basin as well as monitoring, coordinating activities carried by ministries, local government (Provinces and city People's Committee) which may affect to water resources of the basin. Specifically, in the decision No.120/2008/ND-CP issued by the Premier Minister on river basin management, the responsibility of the RBOs becomes very clear, especially their role in solving institutional conflicts.

Basically, the Department of Natural Resources and Environment (DONRE) has similar responsibilities as MONRE, however, at local/provincial scale. Moreover, the DONRE carries out activities under directions of MONRE, but, they are directly controlled by the local/provincial government. Other lower levels (e.g. district or commune) operate within these boundaries. However, at district and commune level, except in some big cities e.g. Ho Chi Minh, Ha Noi, most of officers are not specialized in water resources or even environmental management. Therefore, usually only provincial and national officers have abilities to solve environmental problems.

In addition, there are a number of research institutes and universities as well as companies which are belong or outside MONRE, MARD are cooperating with the government to solve practical problems. International organizations such as UNDP (United Nations Development Programme), World Bank, ADB (Asia Development Bank), JICA (Japan International Cooperation Agency), DANINA (Danish International Development Assistance), BMBF (German Ministry of Education and Research – Bundesministerium für Bildung und Forschung), AFD (Agence Française de Développement), SNV (Netherlands Development Organization), SDC (Swiss Agency for Development and Cooperation) etc. also provides precious assistances to the government.

6.1.4. Monitoring network

As presented in the previous section, the water quality and water quantity was managed by MONRE (i.e. under the Environmental Protection Agency and now as Vietnam Environment Administration) and MARD (i.e. by *Hydro meteorological General Department*). This makes it difficult to combine two data sources as well as utilize data for water resources management. These two agencies are now under MONRE. On 29th January 2007, the Premier Minister issued a Decision No 16/2007/QD-TTg, "Approving the General Planning on the National Network of natural resource and environment monitoring up to 2020". Since then, the harmony between water quality and water quantity has been created. Detailed description on the monitoring program is included in the decision and summarised in Nguyen (2009). Concerning on surface water monitoring, there are some essential points should be mentioned:

- Regarding to surface fresh water monitoring, there are 3 types of monitoring network: (1) environmental monitoring network and (2) Water resources monitoring network; (3) Hydro-Meteorology station network
- The (water) environmental monitoring network includes baseline stations and impact stations. The baseline monitoring network has 60 water quality monitoring points in rivers, 6 water

quality monitoring points in lakes, 140 baseline water quality monitoring points on underground water. The impact monitoring network monitors water quality and solid waste in all 64 provinces and national cities. The list of monitoring stations and points on resources and environment, and the laboratories are planned in accordance with the priority level of the investment (upgraded and newly-developed) in three stages: 2007-2010, 2011-2015 and 2016-2020. Monitoring frequency for the baseline station is at least 1 time per month, and no guide line for frequency of surface fresh water, except impact stations for surface coastal water as at least 4 times per year

- The surface water resource monitoring network to 2020 includes 348 stations, of which 270 station for river water quantity, 116 stations for river and lake water quality. These monitoring stations and points are combined with those of the hydro-meteorological monitoring network. (Table 6.1)
- The hydrological stations (within the Hydro-Meteorology station network) have being constructed based on 248 existing stations. In 2020, there will be 347 stations including upgraded and newly-developed stations (Table 6.1)

Table 6.1: Number of water quality and flow discharge station within the national monitoring program

Water quality			Flow discharge			
Existing	Planned	Total	Existing	Upgraded	Newly-developed	Total
93	116	116	248	123	99	347

The monitoring locations concentrate mainly in environmental hot spots and sensitive areas. The monitoring frequency is four times per year. For the surface water, the monitoring parameters include pH, TSS, turbidity, conductivity, DO, BOD₅, COD, N-NH₄, N-NO₃, P-PO₄, Cl, Total Fe and Total Coliform, and depending on the particularities of each site, other parameters such as heavy metals and pesticide are also monitored.

The national water monitoring program focuses on sensitive and hot-spot river basins e.g. the Cau and Nhue – Day sub basins, Dong Nai – Sai Gon, Ky Cung – Bang Giang, Ca, Huong, Thu Bon, Ba and Mekong river basins. Apart from the national environmental monitoring program, there are many local environmental or water monitoring programs conducted by the provinces (mainly by DONREs). The national/local monitoring programs are gradually improved in terms of number of parameters, frequency and modernization. Supporting budget for monitoring is from central government’s capital as well as local government capital. In addition, monitoring activities are carrying out within a number of research programs. However, these data sources are not well stored and can not collect systematically.

Recently the “minimum water flow” has been introduced as a similar concept to the “environmental water flow” e.g. in the Decree No. 120/2008/ND-CP, 112/2008/ND-CP. The proposed flow aims at utilizing water for demand but still ensuring ecological, environmental preservation. There is also guidance for identifying the flow but it is still very difficult to implement (DWRM, 2009).

6.1.5. Issues in water quality management in Vietnam

Recent efforts from the Vietnamese government have contributed to water resources management. Some typical examples like integrating different institutions, setting up RBOs, identifying polluting companies, releasing more regulatory documents are clearly evidences. However, based on this review, there are a number of issues should be addressed:

- Given the facts of water degradation, the legal and regulatory instruments have been released quite regularly in the recent years. However, these instruments do not really follow up the requirements of water pollution control. In addition, the law is not strict enough to prevent companies from polluting. Even there are companies accept to be fined instead of improving wastewater treatment, for example, maximum fine, in the case of extreme water pollution, is 70.000.000 VND (appr. 3000 Euro) which is much less than constructing, building and operating expensive for a completed wastewater treatment plan (e.g. from 15,000 – 100,000 Euro). Economical instruments are not really implemented e.g. the “Polluter Pay Principle” was mentioned some years ago, however, there is no/limited guidance on this “principle”. Therefore, environmental officers still face many difficulties when dealing with illegal wastewater discharge.
- The institutional conflicts among different ministries or between central government and local ones are relatively solved (i.e. supported by National Water Resources Council, River Basin Organizations). The institutional arrangement seems to be more logically and starts becoming effectively. Their roles have been more clearly recognized. Nevertheless, most of the organization is new; most of the members are not specialized for the Council/Organizations (they have position already in the government). Lacking of staff is also a big issue (e.g. 11 staffs working on water resources protection over 1000km² catchment areas) (MONRE, 2003). Especially, lacking of qualified staffs for the newly-developed institutions (e.g. River Basin Organizations) is also a key issue that makes the progress very slowly. Usually, in-charged staffs only appear when occurring environmental accidents, regular checking is often omitted. The implementing staff is still in progress of “learning by doing” or even “trial and errors” (e.g. allowing operation of wastewater treatment plans which is under accepted levels). Another issue in the “institutional aspect” is ability of public participation in constructing legal documents. Most of the documents are released with very limited consultancy from public that leads difficultly to implement.
- Since the decision No 16/2007/QĐ-TTg has come into implementation, the monitoring data of for surface water can be collected at one institution. Both water quality and water quantity data are in a harmonized fashion so that assessment of water resources becomes more objectively, logically. However, monitoring frequency is still limited. Data collected from other institutions (e.g. DONRE) are not in the same way guided by the Decision (e.g. time, location) that make also difficult to utilize all sources of data. Automatic/real-time water and wastewater monitoring is still on plan and should be implemented as soon as possible.
- Concerning about surface water pollution induced by diffuse sources (e.g. runoff from agriculture activities, urban areas) have not been mentioned in any document. The diffuse source is completely ignored. Especially, in the recent document, the Circular no.:02./2009/TT-BTNMT for regulating assessment of receiving wastewater capacity of water resources, only low flow condition is considered. The high flow, when diffuse sources most often contribute, is not considered for regulating wastewater discharge.

The above discussions have shown some limitations in water quality management in Vietnam. This confirms to the urgent need for finding a suitable tool to the country as already mentioned in chapter 1. Therefore, the aim of this chapter is to propose modeling as a tool to assist water quality management in Vietnam. This assistance will be presented as a model-based water quality management framework

6.2. Model-based water quality management

6.2.1. Modeling tools for water quality management

Mathematical models have been utilized in water resources management in general, in water quality management in particular for a long time. Reviews on reasoning why model is needed can be found in some standard books/reports (e.g. Arheimer and Olsson, 2003; Dzurik, 2003; Hattermann and Kundzewicz, 2009; Loucks and van Beek, 2005; OTA, 1982; Shoemaker et al., 1992; Wurbs, 1994) as already stated in chapter 2, section 2.6.5.

However, in the report of NRC (2001), it states that without or little use of modeling, policy and legislative document can also be established. The example was that many documents, *for example, the Clean Air Act (CAA) of 1967, the Clean Water Act (CWA) in 1977, and the Safe Drinking Water Act of 1976* were released in 60-70s when computer models were not so popular. The only regulatory documents were based on only monitoring data. Nevertheless, some limitations in water resources management were gradually observed (e.g. to link the loop among human activities and natural systems to environmental impacts see Figure 6.2; only controlling point sources, no scenarios development).

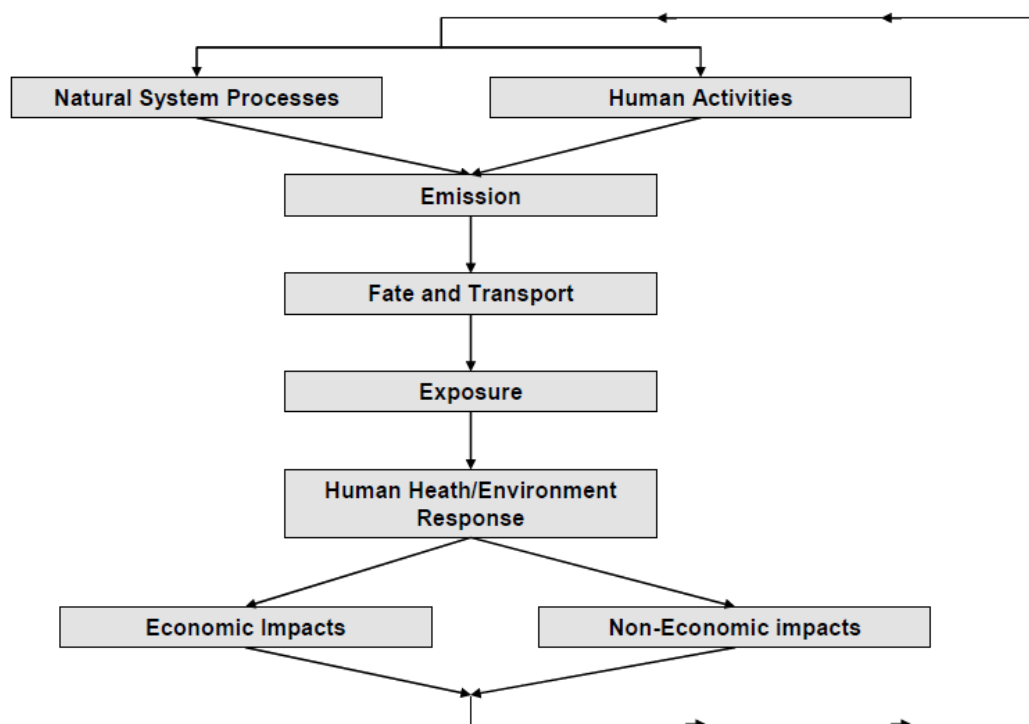


Figure 6.2: Basic modeling elements relating human activities and natural systems to environmental impacts (NRC, 2001)

Therefore, in the Total Maximum Daily Load (TMDL) program, models are extensively utilized later on (Davenport, 2003; Lung, 2001; Shoemaker et al., 2005) as stated in Lung (p.1, 2001) that “*model results are the backbone for a TMDL*”. Similarly, in European countries, Højberg, et al. (2007) state the models can support the Water Framework Directive because it can be used for: (1) Assessment of monitoring data; (2) Interpolation, extrapolation monitoring data; (2) System conceptualization (system understanding); (3) Assessment of anthropogenic activities; (4) Development of management scenarios. In Figure 6.3, Barlebo, et al. (2007) show the model tools may be used at different phases of

the water management processes including designing, implementation, evaluation and identification and it is further illustrated in Figure 6.4 where Kundzewicz and Hattermann (2008) describe more detailed functions of model within each phase of the Water Framework Directive time frame. Especially, models play a particularly important role at the identification, design, implementation and evaluation phase.

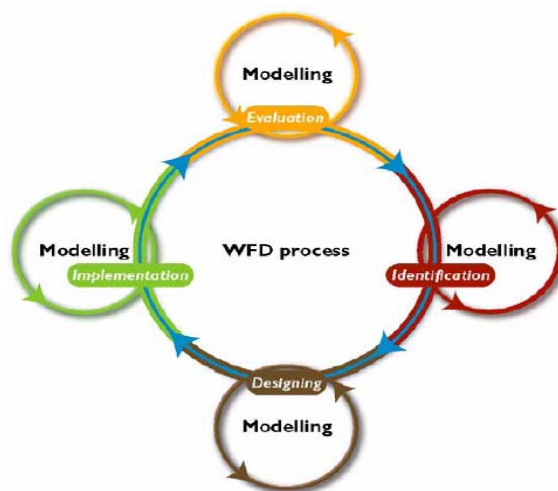


Figure 6.3: Example of the role of a tool (here model codes) in different phases of the water resources management process (the WFD process) (Barlebo et al., 2007)

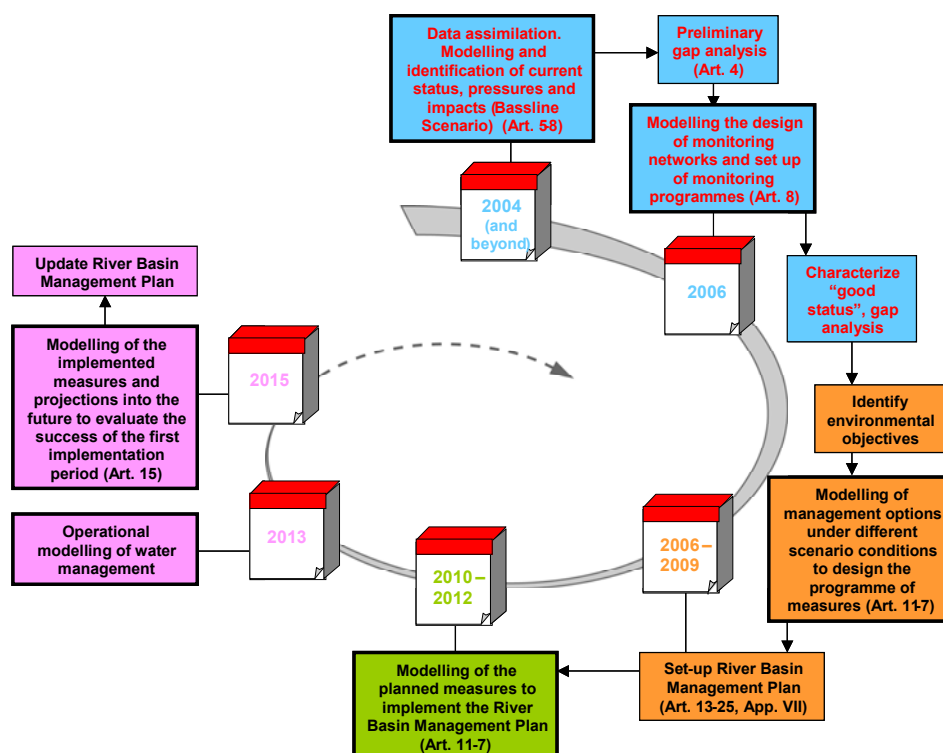


Figure 6.4: Timetable of implementation of the Water Framework Directive and the role of modeling to support different management tasks: identification of pressures and impacts (blue), design of programmes of measures (red), implementation of measures (green) and evaluation of the results (purple) (Kundzewicz and Hattermann, 2008)

Regarding water quality management at catchment scale, model simulation can be utilized in various aspects. There are, for example, integrating different pollution sources (point sources and diffuse sources), implementing at different conditions (low flow and high flow), and adopting to different management strategies (long term and short-term periods). These are explained as follow:

- The point and diffuse sources can be modelled using separated or integrated coupling system (e.g. as presented in chapter 2). The point sources is usually connected directly to receiving water body (e.g. rivers and lakes), while the diffuse sources involve into the whole catchment. In the TDML program, these 2 sources are regarded as waste loads and loads and need to be explicitly presented and will be presented more detailed in section 6.2.2.1.
- The transport and transformation of pollutants coming from these sources depends typically on flow conditions. For example, during low flow period, that means no water supplied from rainfall/precipitation, the contribution of diffuse sources to water body can be ignored, while the effects of point sources can be clearly observed. However, during extreme rainfall events (high flow) the diffuse sources can be a major pollution sources to water quality (i.e. as shown in the modeling work in chapter 4, 5 of this thesis or in Gu and Dong (1998))
- Prediction of water quality variation in short and long-term period is also very important. The short prediction is particularly useful for estimating total pollutant loads in critical conditions (both low and high/extreme flows). This can be used as maximum limits for risk prevention. In another manner, long-term prediction is very essential for water management planning, development of management strategy etc.

6.2.2. Proposing a model-based framework for water quality management in Vietnam

It was proved in the previous sections that modeling is a very useful tool for water quality management and, therefore, it can be very instrumental for Vietnam. In this section, a more in-depth description of what model can assist in water quality management is provided through a number of examples. In addition, relating these aspects with Vietnam conditions is also provided.

To effectively manage water quality at catchment scale, in this thesis, two aspects are considered. They are: (1) Hard solutions (i.e. mainly technological aspects including waste load allocation, water pollution reduction, monitoring) (2) Soft solutions (i.e. perceptional aspects including communication to public participation and decision-maker. The term “hard” and “soft” were used by some authors elsewhere (e.g. in Pahl-Wostl, 2007), however, they are used here as defined above. Figure 6.5 provides a rough model-based water quality management framework that will be discussed in this section. The (waste) load allocation and water pollution reduction will be grouped in section while others are presented separately. The examination of how model support these aspects are carried out by reviewing from literatures.

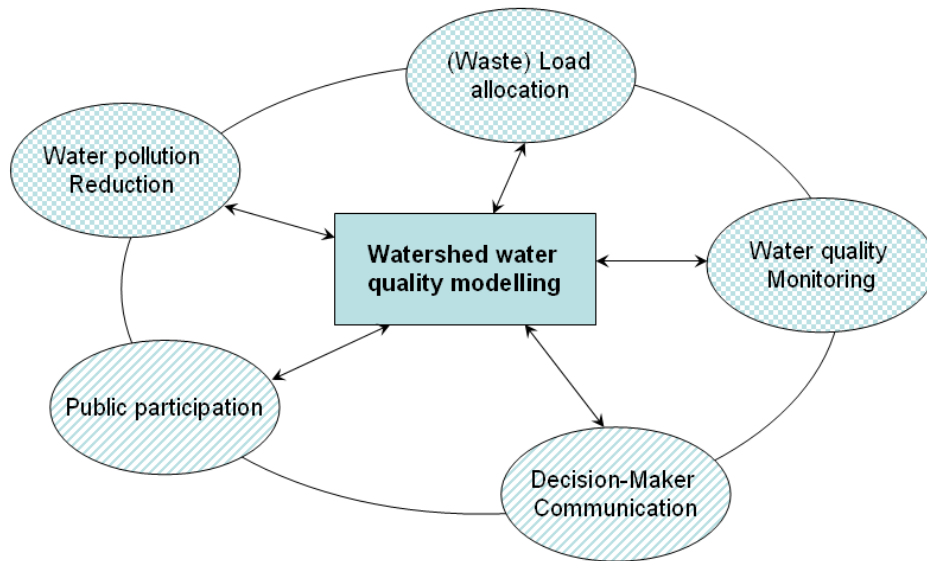


Figure 6.5: A model-based water quality management framework

6.2.2.1. (Waste) load allocation and water pollution reduction

In order to limit pollutants contributing to the receiving water bodies, (waste) load allocation is becoming an effective approach. An example is given to the “Total Maximum Daily Load - TMDL” program (US EPA, 2008). In this approach, load allocation is identified as the contribution from diffuse sources, while the wasteload allocation comes from the point sources and the composed two sources is written hereunder as “(waste) load allocation”. An equation for a TMDL can be generically described as follows:

$$\text{TMDL} = \text{LC} = \text{WLA} + \text{LA} + \text{MOS} \quad (\text{eq. 6.1})$$

Where:

- LC = Loading capacity or the greatest loading a waterbody can receive without exceeding water quality standards;
- WLA = Wasteload allocation, or the portion of the TMDL allocated to existing or future point sources;
- LA = Load allocation, or the portion of the TMDL allocated to existing or future nonpoint sources and natural background; and
- MOS = Margin of safety, or an accounting of uncertainty about the relationship between pollutant loads and receiving water quality. The margin of safety can be provided implicitly through analytical assumptions or explicitly by reserving a portion of loading capacity.

As mentioning previously, Lung (p.1, 2001) states that “*model results are the backbone for a TMDL*” as the load allocation and wasteload allocation can be defined based on model results. Consequently, we hardly see in any TDML development program without the add of modeling tools.(e.g. sediment and nutrient (Borah et al., 2006), bacterial (Benham et al., 2006), dissolved oxygen (Vellidis et al., 2006)). An example of applying the HSPF model for (waste) load allocation is shown in Figure 6.6 where the load and wasteload are allocated at certain volume so that water quality can meet designated criteria or standard.

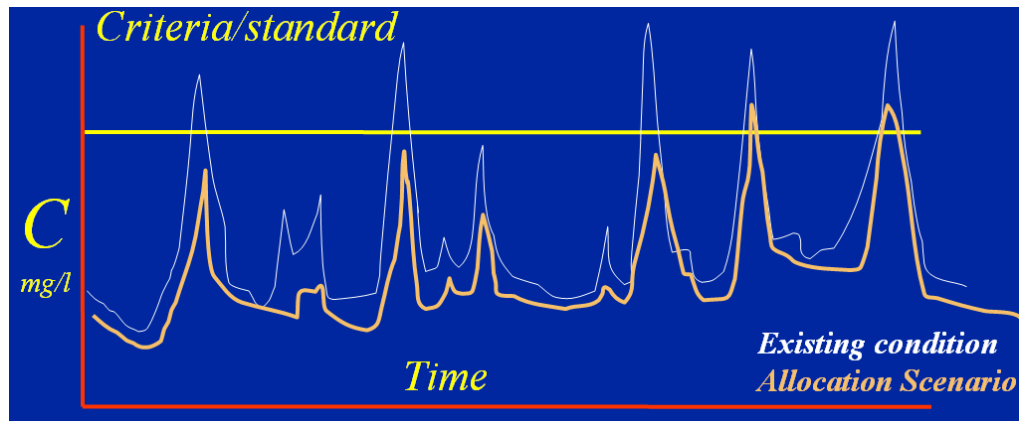


Figure 6.6: An scenario for (waste) load allocation obtained by reducing 20% loading from agriculture, 15% from pasture, 20% from urban and 12% from point sources (US EPA, 2009, lecture 1)

The TMDL is not only supported by deterministic model (e.g. the HSPF, SWAT models), it can be also beneficial based on stochastic approach in order to deal with uncertainty. In Figure 6.7, Novotny (2002) presents how to apply stochastic model to define the TMDL and MOS for water quality protection based on monitoring data. Stow, et al. (2007) combine deterministic-stochastic model to deal with uncertainty aspects in the TMDL program.

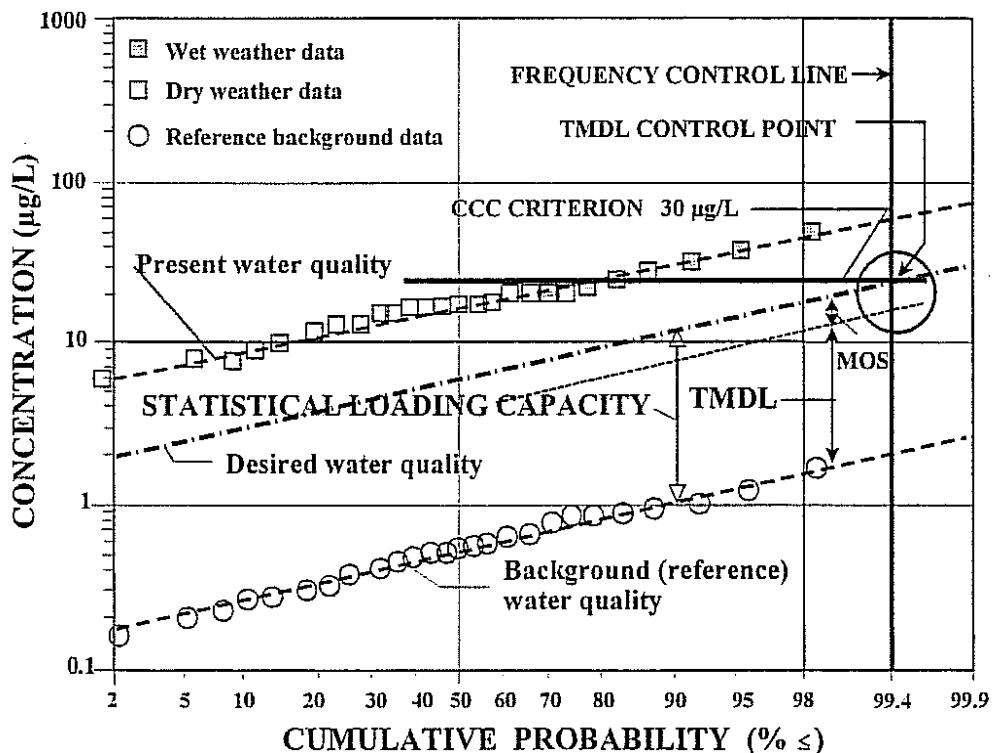


Figure 6.7: Log-normal representation of the monitored data, waste assimilative capacity, TMDL, and MOS. (Novotny, 2002)

Another example on (waster) load allocation is found in the so-called combined emission – immission approach implemented in the European Water Framework Directive (Achleitner et al., 2005; Chave, 2001). In this approach, the emission standard for wastewater discharge is considered together with immission standard which is stand for the capacity of self-purification of the receiving water bodies.

These combined approach will show the required “good water status” and provide upper concentration limits of pollutants discharged from point sources together with other pollutants that come from diffuse sources to water (Chave, 2001). Modeling tools, again, provide good assistances for this approach (Dietrich and Funke, 2009; Hattermann and Kundzewicz, 2009; Horn et al., 2004)

The aim of (waste) load allocation is to ensure the pollutants arrive at receiving water bodies will not be more than the assimilative capacity of the system¹⁴ (i.e. **to prevent water pollution**) so that water can serve as it is prior-designated (e.g. domestic water supply, ecological preservation, irrigation or recreation purposes). In some places, it is impossible to implement the (waste) load allocation since the current waste loads have exceeded the limit of the system (i.e. the water is polluted). In this case, water pollution reduction is required **to restore, improve water quality**. The reduction can be applied for both point sources and diffuse sources (i.e. to reduce pollutants come from point sources and diffuse sources to receiving water bodies) as they are defined in (waste) load allocation. This aspect is related wastewater treatment technology and Best Management Practice. Description on this topic is out of the scope of the thesis that one can refers to some standard documents (e.g. Campbell et al., 2005; Gray, 2005; Kivaisi, 2001; Novotny, 2002; Tchobanoglous et al., 2009). However, the water pollution reduction presented here is to emphasize the links between modeling and engineering techniques applied for cleaning polluted water bodies. Popular techniques are, for example, low-flow augmentation, contaminated-sediment removal or capping, in-stream aeration, restoration of riparian wetlands, and implementation of riparian buffer strips (e.g. (Brix and Schierup, 1989; Chin, 2006; Novotny, 2002))

The effectiveness of water pollution reduction can be incorporated in a catchment water quality model. Some examples are using aquatic macrophytes to reduce lake eutrophication (Bittner, 2008; Xu et al., 1999)), or implementing wetland and riparian to protect water quality (Hattermann et al., 2006; Hattermann et al., 2008). In addition, models can also be useful for operating water treatment system such as a wetland design (Konyha et al., 1995) or wastewater treatment plants (Meon and Le, 2010) . Therefore, similarly to (waste) load allocation as supporting tools, modeling activities can also be instrumental for water pollution reduction.

(Waste) load allocation and water pollution reduction should be defined in catchment planning and regarded as a key solution for water quality management. Management of both point sources and diffuse sources is required in catchment planning. These both technical solutions will help to prevent water pollution and/or to reduce the pollution levels in the water bodies. These are clearly shown in the TDML program (Novotny, 2005; US EPA, 2008) or in the “combined emission – immission approach” guided in the European Water Framework Directive (Achleitner et al., 2005; Chave, 2001). Catchment water quality modeling is particularly useful since it can integrate the (waste) load allocation and water pollution reduction. An example is given to the work carried by Dietrich and Funke (2009) where they present a number of iterative steps in order to incorporate the combined emission-immission approach into a catchment plan by using an integrated modeling system (i.e. the SWAT and RWQM1 models). Figure 6.8 summaries interaction between catchment water quality model and (waste) load allocation, water pollution reduction. The integration of (waste) load allocation and water pollution reduction in catchment water quality model can help to develop various management scenarios.

¹⁴ Cairns (1975) defines *assimilative capacity* as "the ability of an aquatic system to assimilate a substance without degrading or damaging its ecological integrity Novotny, V., 2002. Water Quality: Diffuse Pollution and Watershed Management. John Wiley and Sons, Hoboken, New Jersey, 888 pp.

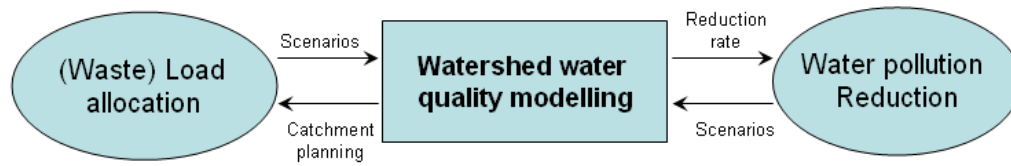


Figure 6.8: Interaction between catchment water quality model and (waste) load allocation, water pollution reduction

Models used for (waste) load allocation can be varied depending on a number of aspects. Typically, they are: data availability, system complexity (e.g. tidal effect, surface water - groundwater interaction, land use discretization, temporal and spatial scale) and expertise. In some case, empirical models can be applied, however, most TMDL programs require complex modeling approach such as HSPF, SWAT, WASP models even integrating or coupling systems have been implemented (HSPF – CE-QUAL W2 (Wu et al., 2006), SWAT – CE-QUAL W2 (Debele et al., 2008), SWAT – MODFLOW (Kim et al., 2008)). Modeling of water pollution reduction often requires experimental treatment (e.g. at pilot scale) and its accompanying models. The treatment efficiency based on experiment can then be integrated with the water quality system of the receiving water bodies or the whole catchment, for example, for river (Meon and Le, 2010), for lake (Bittner, 2008).

In Vietnam, waste (load) allocation is recently directed in the Circular No. 12/2009/TT-BTNMT by Ministry of Natural Resources and Environment on Mar. 19, 2009 regulating assessment of assimilative capacity of water sources for receiving wastewater (MONRE, 2009a). However, in the Circular, the focus is given only for wastewater allocation during low flow period. The circular ignores completely the contribution from diffuse sources although, for example, the existing of these sources during high-flow is illustrated clearly in chapter 4, 5 of this thesis. In addition, the guided appendix of the Circular provides a very simple example that can seriously confuse local officers, scientists.

As far as the author observed, there is no any water pollution reduction projects have been done in Vietnam. There are some plans to restore polluted river by transferring water from other near-by river systems (e.g. Thi Vai (Nguyen, 2008) , To Lich (Long and Binh, 2009)). However, the effectiveness as well as negative effects to ecological system have not been really considered (Quang, 2008) (i.e. not using modeling tools).

6.2.2.2. Monitoring

Monitoring is essential for water quality management. Houlihan and Lucia (1999, cited in Karamouz et al., 2003) categorize the purposes of water quality monitoring as follows:

- Detection monitoring programs are used to detect an impact to surface and groundwater quality
- Assessment monitoring programs are used to assess the nature and extent of detected contaminants and to collect data that may be needed for remediation of contaminants
- Corrective action monitoring programs are used to assess the impact of remediation or pollution control programs on contaminant concentrations
- Performance monitoring programs are used to evaluate the effectiveness of each element of a remediation system in meeting its design criteria

The data provides actual status of water. It is a base for the managers to assess the water quality whether or not sufficient to response to its prior-designated objectives. As mentioned in the Water Framework Directive, monitoring will support the river basin plan where the current status of water throughout the river basin should be taken into account, and is compared with criteria that define the status of the water in the river basin, both in terms of quality and quantity (Chave, 2001). Long-term water monitoring data provides information of variation especially the trend so that the manager can take decisions. However, monitoring alone is not enough when dealing with complex system, especially due to hydrological extremes (flood, drought) and/or under various anthropogenetic impacts (e.g. detection of illegal disposal as presented in chapter 4). System dynamics can not be explained thoroughly by only using monitoring data (e.g. as observed in chapter 3). For this reason, again, catchment water quality models come into play to fill this gap (Jørgensen et al., 2007; Neilson and Chapra, 2003). However, **potentiality of joining water quality monitoring and water quality modeling is not a common practice yet** (Højberg et al., 2007). Therefore, a number of on-going projects are focusing on this issue. For example, Gallé, et al. (2009) in an so-called M3 – “Application of integrative modeling and monitoring approaches for river basin management evaluation”. They (Gallé et al., 2009) are trying to integrate Monitoring – Management – Modeling to support implementing the European Water Framework Directive. Figure 6.9 shows how these three aspects are considered and integrated. In another example, Zsuffa and Pataki (2005) show a guidance of joining monitoring and modeling where monitoring data is accompanied with modeling process (e.g. model building, model set-up, model calibration/ validation) as shown in Figure 6.10.

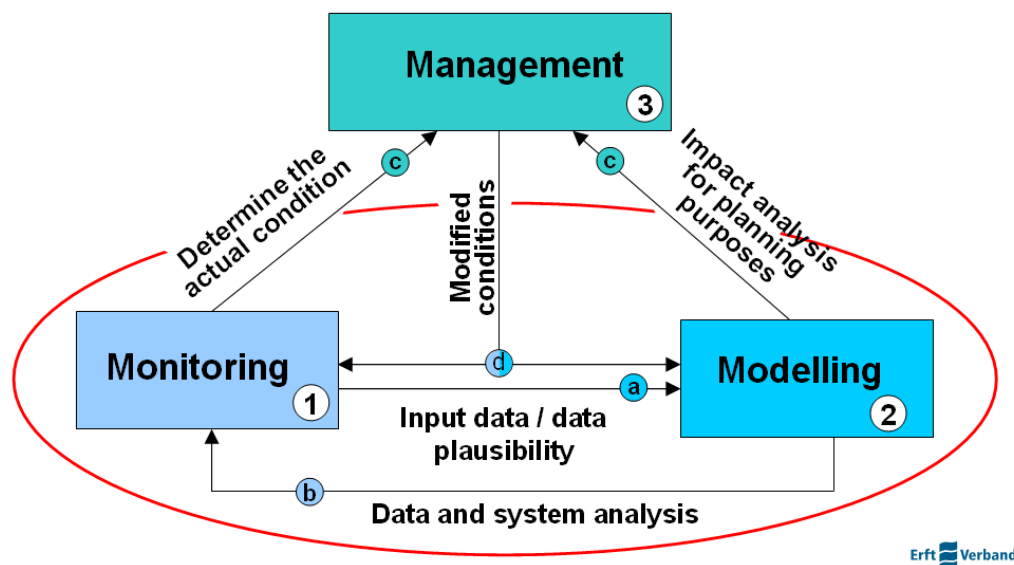


Figure 6.9: Monitoring and model application - M³ concept (Gallé et al., 2009)

Monitoring and modeling are a reciprocal influence. Monitoring data is essential for modeling activities. The data can be input for model simulation, and especially it is used for model calibration and validation (Refsgaard and Storm, 1996). In addition, updated monitoring is very essential for adjusting model parameters (i.e. data assimilation techniques) (Becker et al., 2009; Timmerman et al., 2008) which is becoming a routine practice in real-time forecasting (e.g. flood protection (Madsen et al., 2006)). However, since monitoring is normally expensive, monitoring data is usually not continuously recorded, especially regarding monitoring diffuse sources (Collins and McGonigle, 2008;

lital et al., 2008), modeling become useful to extend measured data. Refsgaard, et al. (2008) list a number of aspect that model can assist monitoring as follow:

- Support for quality assurance of monitoring data. This aspect was also observed in this PhD study where many results of water samples were not used because analyses delayed.
- A “regionalization” tool for interpolation/extrapolation of monitoring data to large areas.
- Support for design of monitoring programmes. This aspect is also observed in the works by Vandenberghe et al. (2007; 2005) where they show modeling was instrumental in designing optimal sampling strategy.

The water quality monitoring activities in Vietnam as well as its limitations has been shown in the first section of this chapter. The current monitoring data in Vietnam is not sufficient enough to carry any in-depth modeling activities. The modeling work can only be implemented within a research project. Thus, data is limited only for short-term simulation. Model-based monitoring is also not found in any documents. Therefore, joining monitoring and modeling in Vietnam will require a lot of efforts in the future.

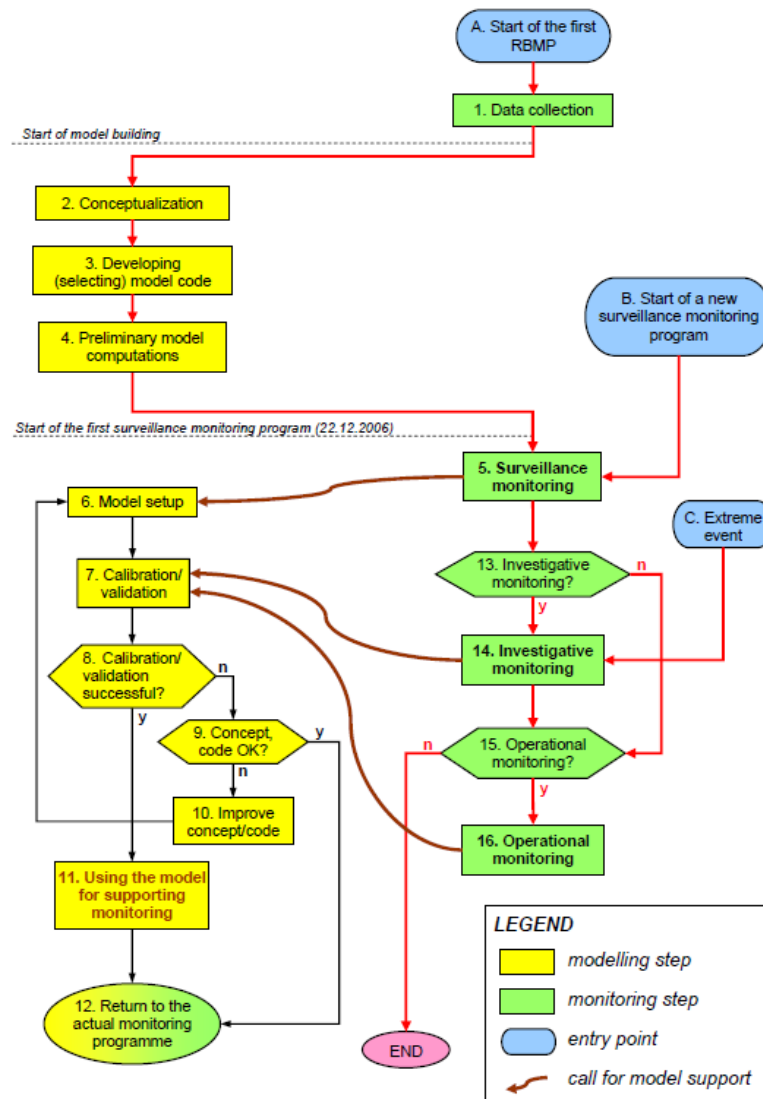


Figure 6.10: Guideline for developing joint modeling and monitoring systems for supporting the implementation of the Water Framework Directive(Zsuffa and Pataki, 2005)

6.2.2.3. Public participation

Catchment processes are very dynamics and complex, thus catchment management in general and catchment water quality management in particular is very complicated. The management is not only limited in technical issues (e.g. induced by physical, chemical, biological processes) but it also relates to political-social-economical aspects (Gooch and Huitema, 2008; Korfmacher, 2001; Pahl-Wostl, 2009). Public participation¹⁵ in water management or community-based catchment management is becoming essential in many water-related projects (e.g. Ridder et al., 2005). Public participation varies at different levels such as global, (multi-) national (e.g. European), regional, local; at different disciplinary e.g. politics, NGOs, scientists, researchers, local citizens (Gooch and Huitema, 2008); at different types e.g. information (i.e. just to be informed), consultation, and active involvement (e.g. co-decision-making) (Pahl-Wostl, 2009). Barth and Fawell (2001) mention that in implementing the Water Framework Directive it is required for peer review and public consultation in order to increase the transparency and uniformity with other directives.

Public participation is very essential in natural resources management and it is also true in catchment water quality management (Pahl-Wostl, 2009; U.S. EPA, 1997; US EPA, 2005). It can be instrumental to water quality management in a number of ways. Typically, they are: (1) Bringing consensus when implementing catchment management plans (NRC, 1999); (2) adjusting and/or adapting environmental policy (Pahl-Wostl, 2007); (3) developing management scenarios (Grizzetti et al., 2008; Newham et al., 2007; Refsgaard et al., 2008). Mostert (2006, cited in Newham et al., 2007) summarises five objectives of participation in catchment management:

- Better informed and more creative decision making
- Public acceptance and ownership of decisions
- More open and integrated management
- Enhanced democracy
- Social learning to enhance management of issues

Public participation and modeling is a bilateral relationship. Public participation can provide consultations on describing system, prioritizing water problems (i.e. targeting modeling objectives), developing scenarios, evaluating model results (Grizzetti et al., 2008; Refsgaard et al., 2008). The most important task from the modeling work in supporting stakeholder is to communicate model results (i.e. answering “What-if” questions). Gooch and Huitema (2008) review on participation in water management including public participation methods that modellers and stakeholders can exchange between each other, especially the “Focus group” method offers a high degree of interactions (Dahinden et al., 2003; Habron et al., 2004).

The aim of this chapter is to illustrate how modeling activities can support in a number of catchment water quality management including public participation. Thus, here how models interact with public participation is illustrated based on 2 examples relating to popular program, the European Water Framework Directive and the TMDL. Kundzewicz and Hattermann (2008), show in Figure 6.11 how model and public participation are involved in river basin planning which is indispensable in implementing the Directive. Furthermore, in step 2 (conceptualization), step 3 (scenario definition and

¹⁵ Here, decision makers are partially included in the public although it is presented separately in the next section.

identifications of management alternatives), step 5 (evaluation of management alternatives) and step 6 (comparison and negotiation) model and stakeholder participatory are accompanied harmonically. Becker, et al.(2009) indicate the interaction between modeller and stakeholder in early planning stage will minimize modeling cost as well as bring modeling result to solve management problems. In another example, Marano et al. (2005) present an integrated approach that stakeholder model and waste load allocation model are involved in a TDML development. They also showed how the technology, economics and decision science are integrated into allocation process and thus communications among all involved parties must be improved.

Model-supported water management

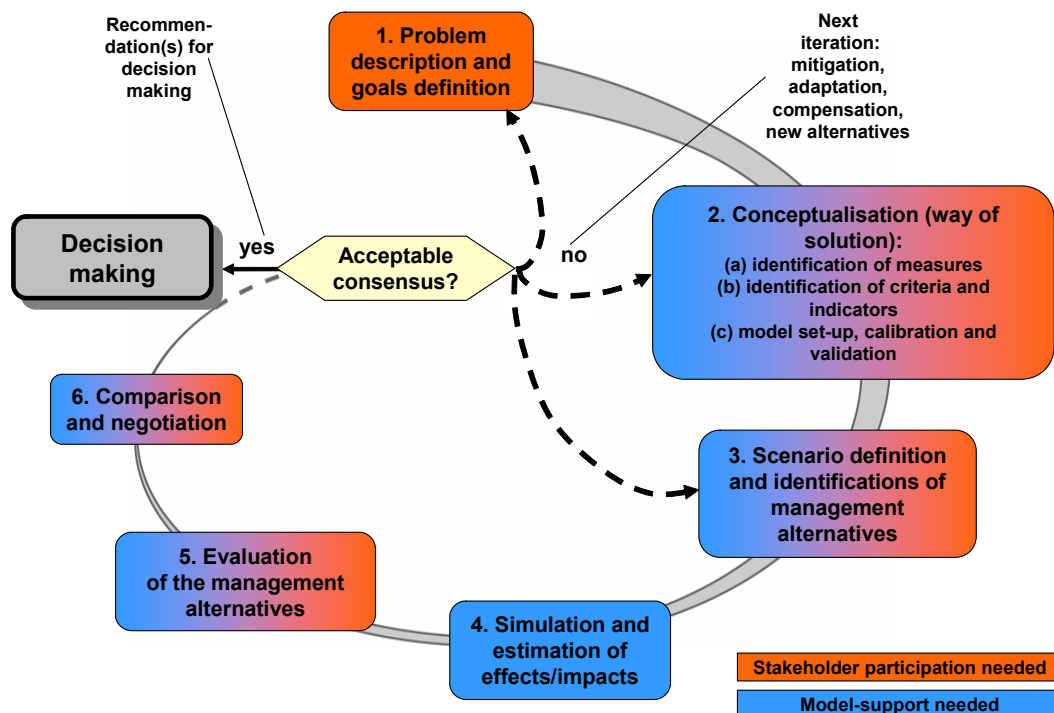


Figure 6.11: Framework for model-supported participatory planning of measures and Integrated River Basin Management (planning framework) (Becker et al., 2009; Kundzewicz and Hattermann, 2008)

Although there are a number of advantages of integrating public participation with catchment water quality modeling as listed above, to implement this approach in practice is not easy (Grizzetti et al., 2008). For example, Korfmacher (2001) identifies several constraints in joining public participation with catchment modeling. They are: (1) Lack of expertise; (2) Risk of biased input; (3) Risk of delegitimization; (4) Risk of overlegitimization; (5) Misrepresenting consensus; (6) Insufficient influence. Thus, he (Korfmacher, 2001) proposed a guideline for involving public participation in modeling activities. The guideline includes five principles:

- Transparent modeling process: The developed or chosen model should be user-friendly, open and flexible and well documented

- Continuous involvement: Public participation should be continuously involved in as many stages of modeling¹⁶ as possible including model development and selection.
- Appropriately representative involvement of stakeholders
- Influence on modeling decisions: the stakeholders should see how their judgements are represented in the decisions.
- Clear role of modeling in catchment management: Model development, modeling results should be clearly informed to both decision-makers and stakeholders

Another guideline regarding technical aspects (e.g. GIS technologies, Free and Open Source Software, Virtual Reality) for enhancing accessibility of modeling tools to non-expert stakeholders that one can refer to the work given by Assaf, et al. (2008)

In the case of Vietnam, Malano et al. (1999) point out “*The law encourages stakeholder participation but has nothing prescriptive to say at all about how or when this will be done*”. It is no evidence about public participatory regarding in modeling processes. It is also confirmed by Matondo (2002) “*Stakeholder participation through public hearing has not been possible in developing countries and this has led to the failure of many water scheme*”.

To conclude for this part, the following paragraph given by Becker et al. (2009) is cited:

*“Integrated management of water resources is a complex task. Successful projects applying models for decision making mostly **have one thing in common**: excellent communication between water managers, modellers and stakeholders. This cooperation allows fitting management to the needs of stakeholders, and models to the needs of water managers. The model setup should be discussed and adapted to the needs of the water managers, and thereby modellers should be so honest to also communicate limitations of modeling.” (Becker et al., 2009)*

6.2.2.4. Communication to decision-maker

Modeling is not only a tool for scientific research but it is also a tool to help decision maker in practice (Savenije, 2009). Dzurik (2003) lists some benefits from modeling activities, for example:

- Mathematical models have significantly expanded the nation's ability to understand and manage its water resources.
- Models have the potential to provide even greater benefits for water resources decision making in the future.
- Models are not explicitly required in any federal water resources legislation, but they are often the method of choice to meet the requirements of legislation

Although in the previous section “(waste) load allocation, water pollution reduction, monitoring” which are already involved in decision-making process, here in section “decision maker”, the focus is given to only two aspects as (I think) these two are the most important with respect to model implementation. They are: Decision support system (DSS) and communicating uncertainty to decision-maker. Other aspects with regarding to legal and regulatory, which are also products of decision-making processes, such as economic tools (e.g. effluent trading, economic incentives),

¹⁶ Korfmacher [2001] presents how public participation involved through 6 modelling steps including: (1) determine objectives, (2) develop a conceptual model of the system, (3) construct the mathematical model, (4) calibrate the model, (5) confirm the model, and (6) apply the model as intended. Or Grizzetti, et al. [2008] show the interactions through (1) model set-up, (2) model validation, (3) model prediction.

agriculture policy (e.g. subsidies, best management practice) are described in some elsewhere (e.g. in Malik et al., 1994; Russell and Clark, 2006; US EPA, 1996; Zhang and Wang, 2002) and are out of the scope of this thesis.

Decision support systems (DSS) are computer-based systems used to assist and aid decision makers in their decision making processes e.g. to find relevant information, accurate summaries, intelligent advice, risk analysis, and to generate, analyze and compare decision alternatives (optimal solutions) (Kersten, 2002; Lam, 2005). Reviews on DSS theory as well as applied in general environment problems can be found in literatures (Jakeman et al., 2008; Kersten et al., 2002) or in some specific water resources problems (Dietrich and Funke, 2009; Lam et al., 2004; León, 1999; Quinn and Hanna, 2003).

The role of modeling in assisting water quality management has been shown clearly above. Again, in a DSS system, models are prerequisite. Kersten (2002) stated that either model-oriented support or data-oriented support, modeling is the critical engine within the system (Figure 6.12). The modeling component can be from a simple model such as empirical, regression equations to a complex model e.g. physically-based, artificial neural networks (e.g. in Lam, 2005; Lam et al., 2004). Models provide quantitative input information resulted from different scenarios to an expert or ranking system together with other input (e.g. map, photo, videos) that will support water managers in a decision-making process. Especially, when dealing with complex water problems, without simulation results, any decision will be very potentially risky (CCSP, 2009). Figure 6.13 is an example showing how water quality models (here, lake model and catchment model are implemented) work within a DSS.

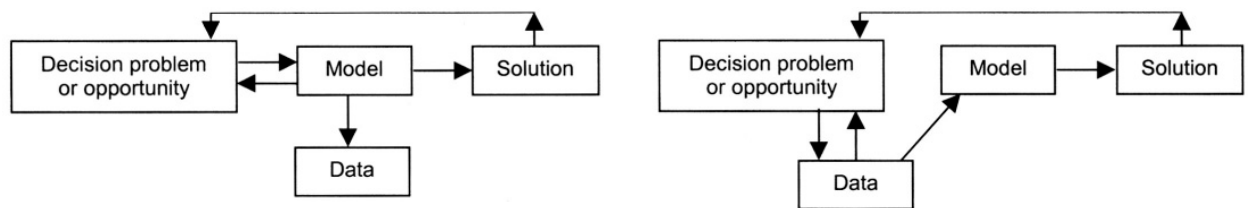


Figure 6.12: Model-oriented support (left) and data-oriented support sequence (right) (Kersten, 2002)

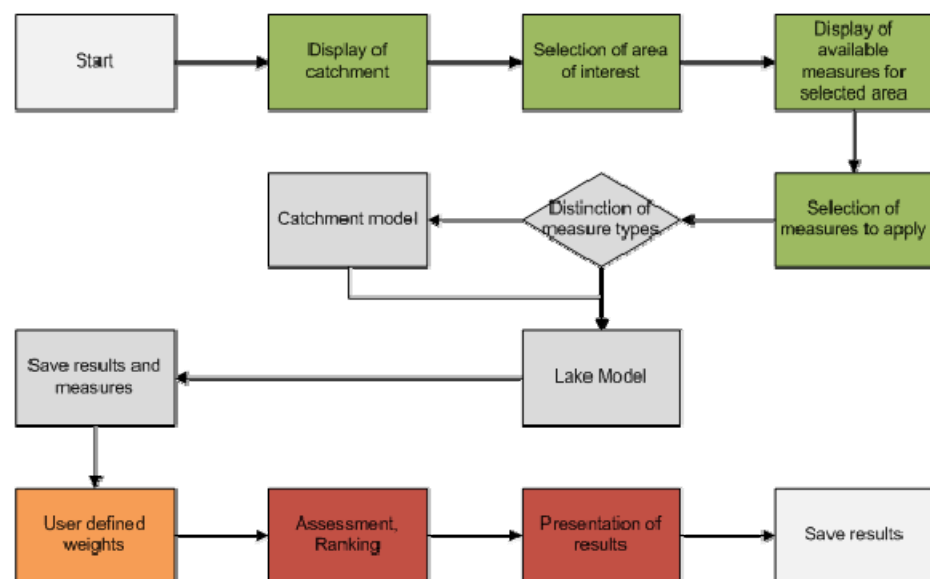


Figure 6.13: The DSS lake Chao (Ruehe et al., 2009)

Based on the above analysis, it is proved that model is a power tool for water quality management. However, as reviewed in chapter two as well as through two modeling exercises in chapter 4 and chapter 5, we must accept that model uncertainty is unavoidable and, therefore, *communicating to decision-maker about uncertainty* must be included (Boffey et al., 1999; Brugnach et al., 2008; CCSP, 2009; Graffy, 1998; Wardekker et al., 2008). This come to a question “how do we communicate this uncertainty to decision-maker (as well as to other stakeholders)?” when they much rely on model results to give important decisions (e.g. Prioritizing management plans, visualising the responsibility of invidual polluter – polluter’s pays principle (Olsson and Andersson, 2007).

In order to answer the previous question, some aspects must be considered: (1) decision-makers’ interests; (2) communication skills. Wardekker et al. (2008) classify different views about uncertainty from decision-maker at different stages in a policy cycle. The decision-makers may look at uncertainty in two ways - either “positivism” or “constructivism” regarding how they interest in the role of science. Therefore, different communication techniques and skills are needed (e.g. in Brugnach et al., 2008; Wardekker et al., 2008). The skills include, for example, convincing decision-maker, providing them useful insights about the existing uncertainty through ways of presentations either qualitatively or quantitatively. However, as pointed out by Wardekker et al. (2008), “Political interest is often limited, and uncertainty adds additional complexity and difficulty in daily practice and in negotiations, and the strategic use”. Therefore, communicating uncertainty to decision-makers still requires a lot of efforts, some guideline e.g. provided by Brugnach et al. (2008), Olsson and Andersson (OTA, 1982), Wardekker et al. (2008) are typical examples for further considerations. A dialogue between manager and modeller given by Hutchins et al. (Hutchins et al., 2006) provide an interesting tool for model evaluation which is presented in appendix 1 of this thesis.

6.2.2.5. Conclusions

In this section, a water quality management framework based on modeling tools has been presented. The support of model has been illustrated in 5 aspects including (waste) load allocation, water pollution reduction, water quality monitoring, public participation, and communication to decision – makers. The framework again proves that modeling tool can be an effective assistance to water quality management. The final part of this chapter will point out some constrains in utilization of models in Vietnam as well provide solutions for future implementation.

6.3. Constraints and solutions for implementing model-based water quality management in Vietnam

It has been proved that modeling is very useful in water quality management. However, there are still a lot of constraints in order to implement in Vietnam. A review on “Constraints to model use” given by OTC (1982) is still valid for Vietnam condition. Those constrains are: 1) *Developing models to meet State needs*; 2) *data limitations*; 3) *lack of qualified personnel*; 4) *access to Federal models*; 5) *reliability and credibility of models*; 6) *model standardization*; 7) *funding*; 8) *maintenance*; and 9) *documentation*. Nevertheless, for the current Vietnamese condition, five generalized aspects are proposed to be considered as the most important ones that cause “constrains to model use”.

- Monitoring data is the most critical issue that has been observed. Although the new national monitoring program have been implemented, there are still several aspects must be considered, for example, higher resolution scale (temporal and spatial scale); insurance of data quality, data integration from different sources.

- Expertise: high qualified scientists as well as management officers are still very limited in Vietnam with regard to understanding model concept, model development and model implementation
- Modeling tools and guidelines: there is no recommended model available for water quality management, especially for management of diffuse pollution. Thus, every institution implementing different models that make difficult to evaluate model results as well as setting up database of model parameters.
- Small scale research study: Small scale study is very important to test and develop model. However, no or limited program for research at small catchment scale exists in Vietnam. A few ones are mostly done within a PhD project and then gone! This leads to difficult to adapt or develop model for Vietnam condition (in order to test the model concepts). Most of the applying models are carried out at provincial or regional scales which are very difficult to understand processes happening inside the areas. This aspects was also discussed for the case of Latin-American countries by in the work of Vegas-Vilarrubia et al. (1994).
- Limited in public participation: As far as I observed, there is no any clear public participation involved into water quality modeling processes except those interviewing activities which is just for input information.

To implement model tools in water quality management in Vietnam, beside the need for improvements of the above constrains, there are several suggesting solutions as follows:

- A comprehensive initiative on water quality modeling program is needed. The initiative should include a wide ranges of studies and applications, for example, for different water domains (e.g. upland, flood plain, estuaries; ground water, surface water); for different problems (e.g. eutrophication; salt water intrusion); different scales (small catchment, river basin). (Examples: BMW (Kämäri et al., 2006), HarmoniQuA projects (Refsgaard, 2002))
- Providing guidance, training so that modeling can become a practice at different institutions. Some examples are given by (Arheimer and Olsson, 2003; Shoemaker et al., 2005; Shoemaker et al., 1997; Shoemaker et al., 1992)
- Operational model is the model that can adapt to site-specific areas. Moreover, the model should not be too complicated to understand and to utilize by local scientists, environmental officer. Therefore, development of a robust model is another important aspect that must be taken into account (e.g. de Blois et al., 2003). An example is given in Lung (2001) where he stated that “Without detailed field data, this (a simple, empirical model namely TVA) predictive methodology was judged to be the best for use in this plan in lieu of a detailed water quality model utilizing questionable assumptions”. This aspect was considered in the report given by the National Research Council (NRC) (NRC, 2007) as “Model Parsimony”. They (NRC, 2007) pointed out the increasing of model complexity in limited data areas can be problematic, and avoiding to add more components that do not improve model performance substantially is preferable. The development of model presented in chapter 5 is an illustration for this suggestion where only important processes were focused.
- One very important issue that must be considered for implementing model in water quality management in Vietnam is uncertainty. An illustration presented in chapter 4 showed that illegal wastewater disposal can contribute a large source of uncertainty in model prediction. In

addition, extreme weather variation makes the model difficult to adapt. Small farming scales also causes certain issues when assigning model parameters or fertilizer input data for different small land use units. Limited data, a critical problem inducing uncertainty, must be improved.

- The adaptive management approach offers a number of solutions for water resources management. This approach has been showing its advantages to deal with complex problems such as uncertainty, public participation, and climate changes (Pahl-Wostl et al., 2007). Figure 6.14 shows a strategy how adaptive management supports water resources management. Discussions on the concept, implementing models in adaptive water resources management can be found in literature (Brugnach and Pahl-Wostl, 2008; NRC, 2004; Shabman et al., 2007; Stow et al., 2007). Therefore, adaptive water quality management should be recommended to Vietnam in the near future.

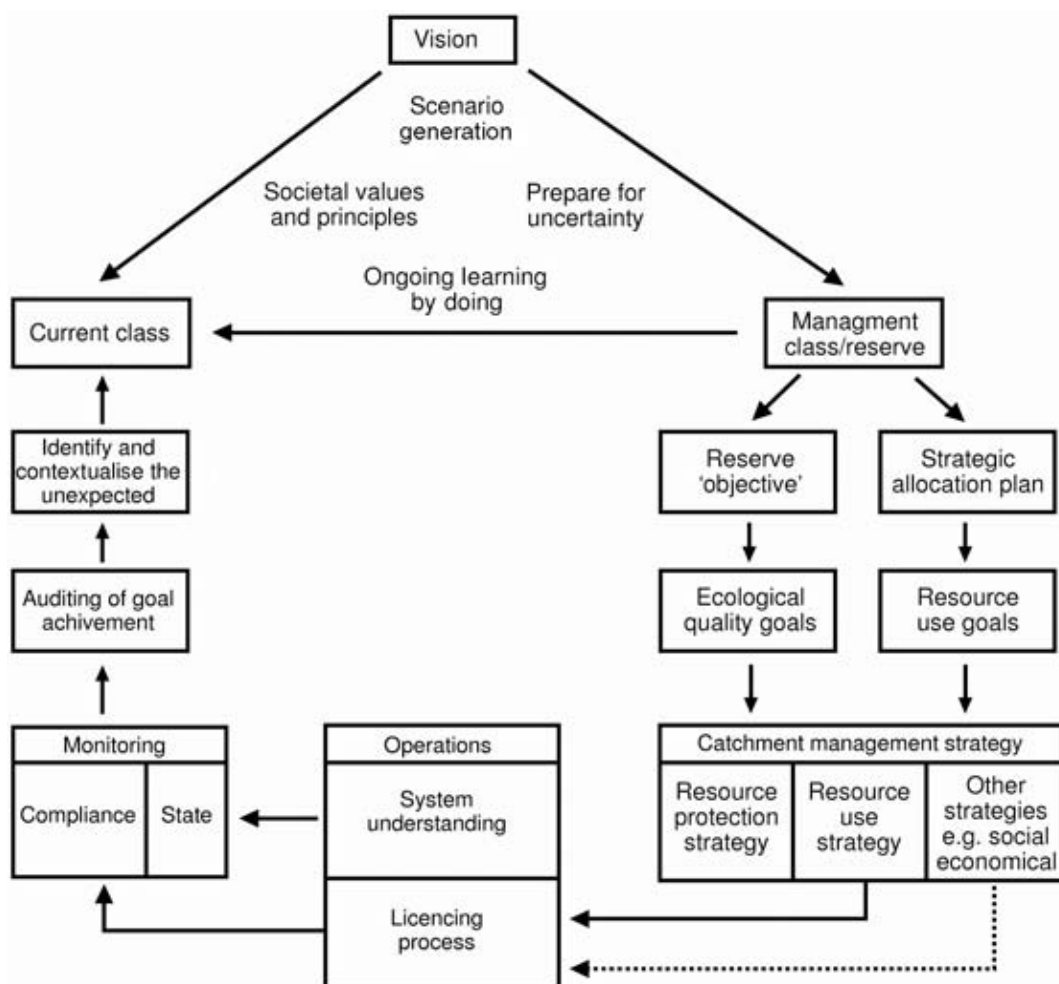


Figure 6.14: Strategic adaptive management of water resources (after Rogers et al., 2000, cited in Newson, 2008, p.353)

7. Conclusions and recommendations

7.1. Conclusions

The aim of this dissertation is the adaption of water quality modeling to tropical regions. The research work was focussed on the modeling of nutrient dynamics due to various anthropogenic factors during flood events. The study has shown an urgent need of utilizing modeling tools for water quality management at catchment scale.

The review in chapter 2 has provided a “State of the Art” of water quality modeling at catchment scale. The review is done in the following orders. Firstly, basic physical, chemical, biological knowledge is provided. It is followed by showing how the processes are represented in model algorithms. Currents issues in water quality modeling at catchment scale (e.g. ungauged catchment, scaling issues, model complexity, model uncertainty, model selection, model evaluation) are also provided that are very important to model implementation and development.

Chapter 3 contains the description of the selected study catchment namely Tra Phi. The catchment is used for implementing and developing models. The chapter includes two main parts: (1) Field survey at Tra Phi catchment; (2) Measurement of river discharge and water quality (focusing on nutrients parameters). The chapter offers an example of how data can be collected in a small catchment in Vietnam under different anthropogenic impacts. Data quality as well as limitations of data monitoring was also emphasized.

Chapter 4 provides an example on how to implement a model. Here one of the most complex catchment water quality models namely HSPF (Hydrology Simulation Program – FORTRAN) was implemented. A review on important physical processes represented in the model is provided. The implementation shows that the HSPF model can be adapted to tropical conditions. The results also show that although the model was successfully applied, many constraints exist due to limited data, parameter uncertainty, expertise requirement etc. that makes the model difficult to be used as operational tool for the region. This aspect is considered for the development of a new model.

In chapter 5, development and test of an event-based catchment water quality SINUDYM model in a robust way to cope with practical issues (e.g. limited data, error propagation) is presented. Simplified model structure and limited model parameters are the most appealing features of the model. All model components are coupled and controlled within one file for use as an operational tool. The model was successfully used to simulate nutrient dynamics at small catchment scale during flood events. For a single event simulation, the SINUDYM provides better results than the HSPF model. Application of SINUDYM confirms the necessity to adapt the model complexity to the data availability of the investigated area.

The aim of chapter 6 was to prove how modeling tools at catchment scale is instrumental for water quality management. Firstly, a review on current water management in Vietnam was provided that leads to the need to develop a model-based water management framework for Vietnamese condition. The framework comprises of (waste) load allocation, water pollution reduction, water quality monitoring, public participation, decision making that all can be beneficial from modeling activities.

Constraints for implementing models in water quality management were pointed out including improving monitoring data, expertise, modeling tools and guidelines, small scale research study, public participation. In addition, recommended solutions for promoting models in water quality management are: developing model-oriented initiative, guidance and training for model development, model implementation, joining integrated water resources management and adaptive water resources management.

7.2. Recommendations

Collected data for model implementation and development were rather limited within the PhD project. More data collection including rainfall, discharge, soil, and water quality is recommended for model validation. This information should be collected systematically and continuously.

For further research on nutrient transport at catchment scale, the same pilot catchment can be used. The research should be focused on, for example, long-term study, nutrient transport mechanism (e.g. at rice field), groundwater and surface water interaction, water quality management schemes (best management practice, wastewater allocation/reduction).

Regarding the group of highly complex models like HSPF, comparative studies using several tropical catchments are recommended. A data bank of parameter sets for the HSPF model under tropical conditions is needed if it is used to support water quality management in the countries.

In order to utilize the new SINUDYM model, e.g. for a long-term prediction, further components – in particular, the ground water contribution, the transport and transformation of nutrient and contaminants in the river need to be added. Furthermore, the program needs to be integrated into a GIS environment.

The main achievement of the author during the PhD phase is the recognition of the role of modeling in catchment water quality management including its limitations. Therefore, the author is looking forward to apply this knowledge for promoting model application in water quality management in Vietnam in the future.

8. References

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1. Appendix 1

Table A1.1: Definitions of a benchmark for three different stages of the model evaluation. (Kämäri et al., 2006)

	Benchmark is a standard	Benchmark is a method of comparison
Model code selection	Specify a fixed set of criteria that can be evaluated against characteristics of the model	Generate an application specific set of criteria that can be evaluated against characteristics of the model
Model performance assessment	Model efficiency(1) should be higher than a predefined benchmark value(2)	Apply a standard model that is generally appropriate and could be used to support the management activity. The efficiency of this model defines the benchmark value. Suitable models should give equal or higher efficiency
A posteriori review of modeling	Specify a fixed set of criteria that can be used to evaluate the contribution of the model in informing the management decision	Generate an application specific set of criteria that can be used to evaluate the contribution of the model in informing the management decision

Table A1.2: Issues and questions in the BMW benchmarking process. (Kämäri et al., 2006)

Issue	Question
Management task definition	<ul style="list-style-type: none"> ▪ What is the problem? ▪ What are the main causes of the problem? ▪ What are the measures that may be implemented to solve the problem?
Model code selection	<ul style="list-style-type: none"> ▪ How well do the model output variables relate to the management task? ▪ Does the model include the key processes relevant to the management task? ▪ Does the model's temporal and spatial span and resolution correspond to the management task? ▪ Are all the necessary data required for the implementation of the model available? ▪ Is there sufficient scientific and stakeholder acceptance of the model code? ▪ Is there sufficient guidance to aid model application? ▪ Has the model code been sufficiently tested? ▪ Does the model code have version control?

	<ul style="list-style-type: none"> ▪ Is the user interface appropriate for the application and user? ▪ How identifiable are the model parameters? ▪ Is there sufficient understanding of the model's uncertainty and sensitivity? ▪ Is the model code sufficiently flexible for adaptation, improvements and linking?
Model performance assessment	<ol style="list-style-type: none"> 1. Is the model's response sufficiently consistent with our understanding of the behaviour of the natural system? 2. Is the assessment of model performance satisfactory? 3. Is the uncertainty in the output of the model application satisfactory addressed?
A posteriori review of modeling	<ul style="list-style-type: none"> ▪ How useful were the model application outputs in informing the management decision? ▪ Was the management action successful in addressing the problem and what did the water quality modeling make a valuable contribution?

Table A1.3: Model Evaluation Tool (Hutchins et al., 2006)

	ISSUE 1: DEFINITION OF THE MANAGEMENT AND MODELING TASK(S)
1.	What is the problem? The water manager defines the problem.
2.	What are the main causes of the problem? 2.1 Make a conceptual model of the problem A <i>conceptual model</i> should help define the interconnections between relevant pressures and impacts and how the problem might be managed. 2.2 Define the broad management objective(s)
3.	What measures may be implemented to achieve the management objective(s) stated in 2.2? List the measures that can be taken to manage the problem. Include options that may provide either a full or part solution to the problem.
4.	GO\NO GO: Is any modeling approach appropriate? Modeling may be appropriate for a partial solution to the management tasks. GO: A modeling approach is appropriate in this case. <i>Finalize the specific management task(s) that can be addressed and choose the model code(s).</i> Proceed to Issue 2. NO GO: A modeling approach is not appropriate in this case. Consider other alternatives
	ISSUE 2: MODEL FUNCTIONALITY AND DATA
5.	Does the model output meet the requirements of the management task(s)?

	<p>Explanation</p> <p>The aim of this question is to determine whether the selected model and its results are useful for investigating the management task(s) detailed in Issue 1</p>	
	<p>Considerations</p>	
	<p>Water Manager</p> <p>What information (model output) is required to investigate the management task(s)?</p> <p>If relevant, do the management scenarios that can be modelled by the chosen <i>model code</i> meet the requirements of the management task(s)?</p>	<p>Modeller</p> <p>Does the model output include the information required to investigate the management task(s)?</p> <p>Which of the management scenarios listed in Question 3 can be modelled by the selected <i>model code</i>?</p>
	<p>Additional guidance</p>	
	<p>Water Manager</p> <p>There may be many mitigation options available. Following dialogue it should become clear which can be modelled by the chosen <i>model code</i></p>	<p>Modeller</p> <p>The information required to investigate the management task may be provided either directly or indirectly via well established procedures</p> <p>Where additional processing is required ensure that sufficient <i>resources</i> are available to enable this to be done</p>
6.	<p>Does the model include the processes and components relevant to the management task?</p>	
	<p>Explanation</p> <p>This question relates to the functionality of a <i>model code</i>, i.e. what the <i>model code</i> can do. Model functionality is determined by the processes and variables that the <i>model code</i> includes. Ideally the functionality of a <i>model code</i> will be balanced with the requirements of a modeling task. Using a <i>model code</i> that contains more process description than required for an application is not a problem if the <i>model code</i> can be used without the additional processes. In some <i>model codes</i> it is relatively straightforward for the modeller to exclude (or include) processes. However in other cases, the modeller is reliant on the <i>model code</i> developer to make changes. A <i>model code</i> is not suitable for a particular application if important processes and/or variables for the management task are not/cannot be included (see Question 17).</p>	
	<p>Considerations</p>	
	<p>Water Manager</p> <p>Describe the key processes and variables required to support the management objective(s). Consider whether you are able to define all the key processes relevant to your application</p> <p>Do you know which management options you want to consider (Question 3)?</p> <p>Consider the <i>resource</i> implications associated with involvement of a third party</p>	<p>Modeller</p> <p>Does the <i>model code</i> include the required processes and are they adequately represented for this application?</p> <p>Is additional functionality / processes representation required? If so, can the functionality be included by the modeller or will a third-party model developer be needed?</p> <p>If necessary, can all relevant management</p>

	model developer	options be incorporated into the <i>model code</i> ? Consider the <i>resource</i> implications associated with involvement of a third party model developer
	Additional guidance	
	<p>Water Manager</p> <p>A complicated description of processes may mean a more extensive demand for input data and <i>resources</i>. This <i>resource</i> demand may be reduced with a less complex, but sufficient, description of processes.</p> <p>Complex models often have greater uncertainties associated with their output</p>	<p>Modeller</p> <p>Identify and highlight situations where the <i>model code</i> representation may be inadequate for the current application</p> <p><i>Model codes</i> sometimes claim to include certain processes and management options, but in reality their ability to represent these processes is limited by the model structure</p> <p>Although simple <i>model codes</i> may not include important processes explicitly, these may be implicitly represented, for example, in the form of an empirical relationship. Consider if this form of representation is adequate in the context of the management task.</p> <p>Processes not required for the <i>model application</i> may be turned off if there is no impact on model calculations. This may reduce prediction uncertainty.</p> <p>If necessary, consider linking models from different domains, e.g. socioeconomic and bio-physical models.</p>
7	<p>Does the temporal and spatial span/resolution of the <i>model code</i> correspond to the management task?</p> <p>Explanation</p> <p>Choosing an appropriate temporal and spatial scale/resolution at which to investigate a management task is crucial and should be conducted before initiating a modeling exercise. The WFD requires management plans to be developed at the river basin scale. The spatial resolution of a basin-wide <i>model code</i> can range from lumped (a single unit, the basin), to semi-distributed (the basin divided into several sub-basins) and fully distributed (the basin divided into a grid), depending on what is required to solve the problem. It may, however be necessary to model isolated systems. In order to gain full insight into the processes affecting a system, hourly, daily, monthly, seasonal or annual differences might need to be investigated. An appropriate temporal resolution is also dependent on the specified management task(s) (Issue 1).</p>	
	Considerations	
	<p>Water Manager</p> <p>Discuss the required temporal and spatial spans/resolutions at which the <i>model code</i> should be applied to meet the requirements</p>	<p>Modeller</p> <p>Determine whether the <i>model code</i> can operate and provide output at the required temporal and spatial spans/resolutions. Consider (1) the</p>

	<p>of the management objective (Question 2.2)?</p> <p>Consider the temporal/spatial characteristics of the processes to be modelled, including management options/ measures (Question 3).</p> <p>Given the management task, will the <i>model</i> output be used by other <i>models</i> and/or will the <i>model</i> be using output from another <i>model</i> as input.</p>	<p>objectives of the study, (2) the temporal dynamics of the processes to be modelled, (3) the spatial representation of the processes to be modelled, (4) data availability</p> <p>In the case of linked/integrated modeling, consider whether the selected span and resolution are still appropriate for the application</p> <p>Consider the feasibility of defining <i>boundary conditions</i> and <i>initial conditions</i>. This may not be straightforward for <i>model codes</i> of high spatial/ temporal resolution.</p>
	Additional guidance	
	<p>Water Manager</p> <p>Unnecessarily complicated, as well as unnecessarily simplified models should be avoided.</p> <p>More detailed descriptions of processes in time and space can mean a more complicated modeling process.</p> <p>This may result in (1) larger uncertainty in model outputs, and (2) <i>resource</i> implications.</p>	<p>Modeller</p> <p>The temporal resolution of the <i>model code</i> should be in good agreement with the temporal characteristics of the processes to be modelled</p> <p>A detailed spatial representation of the basin would suppose that appropriate aggregation algorithms are available to provide <i>model</i> output at the basin scale</p> <p>Data availability may constrain the choice of <i>model</i> resolution, especially if real time management applications are concerned.</p> <p>Spatial and temporal resolution should be chosen in agreement with the available financial <i>resources</i> of the end-users.</p>
8	<p>Are the data required for the implementation of the model available?</p> <p><i>Explanation</i></p> <p>This question relates to the balance between the input data requirement of a <i>model code</i> and the input data available for the <i>model application</i>. Input data are quantitative or qualitative values that are required to carry out the <i>model</i> simulation. Lack of available input data can hamper the practical application of a <i>model code</i>. The optimum case is when all essential input data are available from monitoring and/or field observations (primary data). Secondary/surrogate data (data from other <i>model</i> runs, other nearby sites or literature) can be used to supplement the primary data. However, if the majority of the data required for an anticipated <i>model application</i> is secondary, or if essential data is still missing use of <i>model code</i> should be carefully considered. Gaps in input data can have an impact on <i>model</i> output.</p>	
	Considerations	
	<p>Water Manager</p> <p>What data are available for the region?</p> <p>What are the <i>resource</i> requirements for obtaining extra data?</p>	<p>Modeller</p> <p>Are there sufficient input data available to enable the <i>model application</i> to produce the required outputs?</p> <p>Consider whether the scale and resolution of available data are appropriate.</p>

	Additional guidance	
	Water Manager If relevant, describe the source and reliability of the data	Modeller Some data required for the <i>model application</i> may be generated from other models, as opposed to primary sources. Filling gaps in data will require assumptions to be made and may affect local variability/predictions. Be aware of data quality, reliability, quality assurance and provenance etc. Given data availability a <i>model code</i> may be insufficient for the entire <i>model application</i> . However, it may be adequate for part of the application and could be used in conjunction with expert knowledge or as part of a linked <i>model application</i>
9	GO\NO GO GO: The selected model code is potentially suitable for this management task NO GO: The selected model code is not suitable for this management tasks. Return to question 4	
10	Is there sufficient scientific and stakeholder acceptance of the model code? Explanation This question is directed towards the documentation, acceptance and reputation of the science behind the model code among the (international) scientific community. It focuses on the structure of the model code and how the conceptual model behind the model code fits with established scientific theory in its domain. It is also very important to consider the credibility of the modeller. The manager may have little expertise/Awareness of modeling. This question is related to question 12	
	Consideration	
	Water Manager Is the technical documentation assessable and easily understandable? Can the technical documentation be used to underpin the results of the study? Is it important that the scientific content underlying the model code is published in peer review journals? Is it important that the model code has been used in decision making application? Do you believe in this model (question 12)?	Modeller Is the <i>model code</i> sufficiently known and scientifically accepted? Consider (1) peer-reviewed publications in scientific journals, (2) the degree of acceptance/use of the <i>model code</i> within the scientific community, and (3) whether the <i>model code</i> has been used in other policy decision making applications? Is there a technical document available that provides a comprehensive detailed description of the theory, processes, equations, algorithms, and numerical methods include in the <i>model code</i> or can you obtain addition information via other sources

	Additional guidance	
	<p>Water Manager</p> <p>Will you need to justify the model application, the model code and the science behind the model code to end user?</p> <p>Will you need assess to adequate written documentation on the equations, theory, numerical techniques etc. of the model code?</p> <p>Newly developed model code may not have been published widely. This does not reflect badly on the quality of science behind the model code</p> <p>Unsuccessful applications of model code are not often reported</p>	<p>Modeller</p> <p>A large number of publications may suggest good science but this should not be only consideration.</p> <p>Newly developed <i>model codes</i> may not have been published widely. This does not reflect badly on the quality of science behind the <i>model code</i>.</p> <p>Will additional documentation need to be prepared before delivery?</p>
11	<p>Is there sufficient guidance to aid model application?</p> <p><i>Explanation</i></p> <p>Unless the <i>modeller</i> is very familiar with the <i>model code</i>, the set-up, understanding and proper application of a <i>model code</i> requires clear and up-to-date user instructions. Moreover, a tutorial with application examples (preferably with test case data) is a very useful tool to demonstrate the functioning of the <i>model code</i> to a new user. Even if the <i>modeller</i> is familiar with the <i>model code</i>, for model results to achieve credibility amongst the water manager and stakeholders it is important that they can gain insights into how the <i>model code</i> functions, along with its capabilities and limitations.</p>	
	Considerations	
	<p>Water Manager</p> <p>Do you need a detailed well-organized user manual for the <i>model code</i> either now or in the future?</p> <p>Would application examples be beneficial?</p> <p>Are they available and useable?</p>	<p>Modeller</p> <p>Is there an up-to-date, comprehensive, operable and clear user manual for the <i>model</i>?</p> <p>Is there a useful tutorial and application example(s) with test datasets?</p> <p>Is it easy for you to explain the modeling process and results to the water manager?</p>
	Additional guidance	
	<p>Water Manager</p> <p>Do you want to own and use the <i>model code</i> and application yourself for future purposes?</p>	<p>Modeller</p> <p>Are the scope of the model, its application domain, file structure, and <i>parameter</i> estimation methods fully explained?</p>
12	<p>Has the model code been sufficiently tested?</p> <p><i>Explanation</i></p> <p>Past experience can provide some indication as to the quality of a <i>model code</i>. However,</p>	

	<p>unsuccessful applications are rarely reported. In general, it is preferable if a <i>model code</i> has previously been tested under similar conditions or if it has proved to be reliable over a large number of applications. The transformation from conceptual model to <i>model code</i> should also be considered here. Errors may have occurred during transformation. Any errors may have since been fixed, increasing the credibility of the <i>model code</i>,</p>	
	Considerations	
	<p>Water Manager</p> <p>Do you require a formal measure of reliability, e.g. for quality assurance purposes and/or trustworthiness of results?</p>	<p>Modeller</p> <p>What testing has been conducted in order to ensure the trustworthiness of the <i>model code</i>?</p>
	Additional guidance	
	<p>Water Manager</p> <p>There is no guarantee that a <i>model code</i> will work properly for a new application even if it has been tested for several similar applications.</p>	<p>Modeller</p> <p>Successful applications on other applications, even if very similar, can not be considered as an absolute guarantee of <i>model</i> reliability for a specific application.</p> <p>Has there been any code review?</p>
13	<p>Does the <i>model code</i> have version control?</p> <p><i>Explanation</i></p> <p>Refinements, modifications and other changes, e.g. bug-fixes, that are made to the <i>model code</i> can change the behavior of the <i>model</i>. Therefore, it is important that a version number is attached to the <i>model code</i> and that this number is updated when new revisions to the <i>model code</i> are made. Changes and their implications should be properly explained in model documentation.</p>	
	Considerations	
	<p>Water Manager</p> <p>Do you require version control?</p>	<p>Modeller</p> <p>Are the different model versions traceable and do they contain descriptions of any modifications?</p> <p>Does the available user manual and other documentation match with the model version under consideration?</p> <p>Is this clearly indicated?</p>
	Additional guidance	
	<p>Water Manager</p> <p>If necessary, ensure that the modeller can provide information on the version of the <i>model code</i> to be used.</p> <p>Be aware that different versions of the same <i>model code</i> might produce different results</p>	<p>Modeller</p> <p>Bear in mind that you might be reliant on the quality of the documentation of version control as provided by the model developer?</p>

14	<p>Is the user interface appropriate for the application and user?</p> <p><i>Explanation</i></p> <p>Lack of understanding of the modeling process and/or poor communication of modeling results can lead to misunderstanding, frustration and unrealistic expectations. Dialogue, interaction and mutual understanding are therefore important for enhancing the credibility of <i>model</i> results in decision-making. Correct understanding of the modeling process and model output is important for making the right decisions. An easily understandable user interface and output can facilitate the decision making processes</p>	
	<p>Consideration</p>	
	<p>Water Manager</p> <p>Does the model have an informative user interface with easy visualisation of the output?</p> <p>Does the modeling process and the presentation of results allow for effective negotiation amongst stakeholder</p> <p>Do you expect the acceptance of the results to be dependent on the under standing of the modeling process?</p> <p>Will a non-specialist need to interpret the scenarios, or initiate further analyses? Note this does not mean that everybody should be able to set up and use the <i>model</i>?</p>	<p>Modeller</p> <p>In what forms can you present the model output and are they easily understood?</p> <p>Is the user interface easily understood and navigable?</p> <p>Is the <i>model code</i> well structured and does it allow for (1) end-users to do straightforward subsequent analysis, e.g. scenario analyses, and (2) an easily interpretable presentation to stakeholders?</p> <p>Is active user support available either from model developers or from a user-group?</p>
	<p>Additional guidance</p>	
	<p>Water Manager</p> <p>GIS representation of results can be misleading due to, for example, interpolation between points.</p>	<p>Modeller</p> <p>It is not expected that everybody should be able to set up and use the <i>model</i>.</p>
15	<p>How identifiable are the model parameters?</p> <p><i>Explanation</i></p> <p>This question relates to representation of the processes described in the <i>model code via model parameters</i> (the numerical values that control the model processes).</p> <p><i>Parameter</i> values are usually identified partly via <i>calibration</i> and partly by taking values from the literature and/or earlier experience. In general, the more a <i>model code</i> is based on 'true' description of processes (physically-based) the more closely related the <i>parameters</i> tend to be to physical/chemical biological phenomena. For physically-based <i>model codes</i> therefore it should be possible to relate many model <i>parameters</i> to field measurements of physical properties. In contrast 'black-box' <i>model codes</i> contain <i>parameters</i> that cannot be observed and are generally specific to a particular <i>model code</i>. These <i>parameter</i> values are determined purely by <i>calibration</i>, although ranges of variation are often given. Uncertainty in model <i>parameter</i> values can lead to equifinality of model prediction, whereby for a specific set of input data more than one distinct set of <i>parameter</i> values can generate simulations characterized by equally optimal performance criteria</p>	

	Consideration	
	Water Manager Is a measure of uncertainty required, e. g. for risk based assessment?	Modeller Do model <i>parameters</i> need to be calibrated? How valuable are <i>sensitivity analysis</i> (determining crucial model inputs) and <i>uncertainty analysis</i> (studying uncertainty of model outputs) in verifying the quality of a model?
	Additional guidance	
	Water Manager	Modeller Detail (if any) specific requirements in terms of model parameterisation, e.g. identifiability Identification of <i>parameter</i> values can be a difficult procedure. The resulting values of calibrated <i>parameters</i> are not necessarily accurate. It is possible that a chosen and acceptable calibrated set of <i>parameters</i> may later be deemed to be of suspect accuracy after subsequent and more detailed analysis of model output.
16	Is there sufficient understanding of the model's uncertainty and sensitivity? <i>Explanation</i> <i>Sensitivity</i> (SA) and <i>uncertainty analysis</i> (UA) are important parts of a modeling study. SA can be used to reduce the number of model <i>parameters</i> aiding <i>calibration</i> whilst UA can be used to help a decision-maker judge whether modeling results are sufficiently precise to support decision-making. This questions aims to evaluate how easily a <i>model code</i> can be implemented in a SA and/or UA analysis framework.	
	Consideration	
	Water Manager Is information on the most sensitive <i>parameters</i> in the application required? How valuable is information on uncertainties in connection with the modeling results? What <i>resources</i> are available for conducting SA and UA?	Modeller How can SA and UA be implemented to/in the <i>model code</i> to run analyses for this application? Is it feasible to run the model hundreds of times with varying input data and <i>parameter</i> values? Is it feasible to produce SA and UA assessments given the <i>resources</i> and deadline for the application?
	Additional guidance	
	Water Manager SA and UA may help in the discussion with other end-users about reliability of modeling results.	Modeller SA and UA techniques may not be easily applicable or user friendly. Have SA and UA been conducted during

	<p>The results of sensitivity analyses are not always straightforward to interpret, guidance from the modeler might be necessary.</p>	<p>previous applications of the model code?</p> <p>Results of SA and UA are not always straightforward to understand/interpret, e.g. con-elation between variables might not show up clearly in SA, making interpretation of results difficult.</p>
17	<p>Is the <i>model code</i> sufficiently flexible for adaptation, improvements and linking?</p> <p>Explanation</p> <p>In many modeling applications there will be some need for modifications or customizations to be made in the model code. Difficulties in gaining access to and/or understanding the model code may hamper development. A third party modeller or model developer may be required to make changes under these circumstances. In addition there may no longer be persons/organizations active in the model's development.</p>	
	<p>Considerations</p>	
	<p>Water Manager</p> <p>What resources, if any, are needed to support further development of the model code to improve its suitability for this application?</p>	<p>Modeller</p> <p>Do modifications need to be made to the model code to improve its suitability for this application?</p> <p>Is the model code tlexible, i.e. different processes can be made active or passive in the model application using add-on modules or switches?</p> <p>If the model source code is available to the model user, is it well structured and documented?</p> <p>If the model source code is not generally available, will the developers be prepared to give support for adaptation and improvements?</p> <p>If required, can the model code be easily adapted for inclusion in an integrated model system?</p>
	<p>Additional guidance</p>	
	<p>Water Manager</p> <p>Further development may be necessary to make a model code suitable for application in different catchments.</p> <p>Model code adaptations can be resource intensive.</p>	<p>Modeller</p> <p>Are you able to adapt the model code yourself reliably, or do you need external help?</p> <p>In some cases the model code may need to be linked/chained to other model codes in order to define over all results, i.e. model code should become part of an integrated model?</p>
18	<p>GO / NO GO: Is the <i>model code</i> suitable for this application?</p> <p>GO: Apply the selected <i>model code</i> for the application.</p> <p>NO GO: Consider returning to either Question 4 (evaluate a new model) or</p>	

	Question 9 (evaluate the same model but consider if relaxing criteria), as appropriate.	
	Water Manager	Modeller
	ISSUE 3: MODEL PERFORMANCE ASSESSMENT	
19	<p>Is the <i>model application</i> response sufficiently consistent with your understanding of the behaviour of the natural system?</p> <p>Explanation</p> <p>The <i>model application</i> must be able to describe the current situation in a coherent way, consistent with accepted scientific understanding. The simulation results will gain credibility when the response of the model to changes in the input can be understood intuitively and can be explained logically. This may be hard to evaluate when the <i>model application</i> concerns a complex, poorly understood system. In such cases the modeling process may be important in terms of gaining insight regarding system behaviour.</p>	
	Consideration	
	<p>Water Manager</p> <p>Is the setup of the <i>model application</i> realistic?</p> <p>Do the simulation results fit with common sense?</p> <p>Has the model code gained its credibility for a situation similar to your study area? The answer to Question 12 should also be considered?</p>	<p>Modeller</p> <p>Has experience gained in previous studies with the <i>calibration</i> of the <i>model application</i>? The answer to Question 12 should also be considered.</p> <p>Consider the temporal variations in the model output (daily, seasonally) in response to changes in the pressures</p> <p>Consider the spatial variations in the model output (locally, regionally) in response to geographical changes in the pressures.</p> <p>Is the number of <i>calibration parameters</i> realistic, compared to the number of output variables? (over parametrization)</p> <p>Are the calibrated model coefficients within a realistic range?</p>
	Additional guidance	
	<p>Water Manager</p> <p>Check whether the <i>model application</i> confirms your ideas about the behaviour of the natural system</p> <p>The model should be credible both for the current situation and the future situation</p> <p>The behaviour of some very complicated systems can only be studied via models, e.g. the climate system.</p>	<p>Modeller</p> <p>Discuss the behaviour of the <i>model application</i> with domain experts.</p> <p>Be aware that in the case of overparameterized models statistically good <i>model performance</i> can be obtained using an unrealistic description of the system (via unrealistic values of calibrated <i>parameters</i>).</p>
20	Is the assessment of the <i>model application performance</i> satisfactory?	

	<p>Explanation</p> <p>The <i>model performance</i> is the goodness of fit of the simulation results with the measured data. The <i>model performance</i> must be good enough for decision making. This involves agreeing (before <i>model application</i>) on performance criteria for <i>model performance</i> assessment and a quantitative definition of what level of performance constitutes being "good enough"</p>	
	<p>Considerations</p>	
	<p>Water Manager</p> <p>Have data sets been used for <i>validation</i> of the model that are independent of datasets used for model <i>calibration</i>?</p> <p>Is the situation for which the model has been calibrated comparable to that for which the model will be used to evaluate measures?</p> <p>Is the <i>model application performance</i> good enough for decision making? What are the consequences if a decision is made on the basis of inaccurate model results? Consider whether any subsequent changes in the environment and society are irreversible?</p>	<p>Modeller</p>
	<p>Additional guidance</p>	
	<p>Water Manager</p> <p>Define realistic goals for the model <i>calibration</i> that are agreed upon before the <i>calibration</i> phase of the study starts.</p> <p>Modellers tend to show the best <i>calibration</i> results, therefore ask for the output that is not presented.</p>	<p>Modeller</p> <p>Define realistic goals for the model <i>calibration</i> that are agreed upon before the <i>calibration</i> phase of the study starts.</p> <p>Be aware that techniques such as regression analysis may be insufficiently rigorous for the specific application. Their use could create a false sense of security</p> <p>Discuss and agree upon the methodology to be applied.</p> <p>Bear in mind that statistically good <i>model performance</i> should only be acceptable when calibrated model coefficients hold realistic values</p>
21	<p>Is the uncertainty in the output of the <i>model application</i> satisfactory addressed?</p> <p>Explanation</p> <p>The output of a <i>model application</i> is subject to uncertainty because of several reasons. Lack of input data, simplifications in the <i>model application</i> and natural variability tend to decrease the certainty of the model output. The confidence in the <i>model application</i> depends on the (un-) certainty of the model output.</p>	
	<p>Consideration</p>	

	<p>Water Manager</p> <p>Is the suggested method for <i>uncertainty analysis</i> generally accepted both scientifically and by end-users?</p> <p>Have all uncertainty aspects that are of importance for the decision making process been addressed?</p> <p>What level of certainty of the model results is needed for decision making?</p> <p>In the light of assessments of uncertainty in model output discuss with the modeller whether the <i>model application</i> be used with confidence to inform management decision-making</p>	<p>Modeller</p> <p>Consider whether the uncertainties are specific for the study area, or for a larger region. How likely are these uncertainties in your study area?</p> <p>Can the uncertainty in the model output be reduced significantly, with a limited amount of extra effort? (What is the cost-benefit ratio of reducing the uncertainty in the model ling study?)</p> <p>Demonstrate whether the impact of any predefined management scenarios on model output is greater than the uncertainty associated with the model output itself. If not discuss with the water manager how this outcome reflects on both the nature of the scenario and the uncertainties associated with the <i>model application</i></p>
	Additional guidance	
	<p>Water Manager</p> <p>Note that uncertainty does not include the modeling concept (you don't know what you don't know).</p>	<p>Modeller</p> <p>Discuss and agree upon the methodology</p> <p>Check: www.harmonirib.com</p>
	ISSUE 4: A POSTERIORI REVIEW	
22	How useful was the <i>model application</i> for informing the management?	
	Considerations	
	<p>Water Manager</p> <p>Was it possible to make a decision the basis of the modeling results?</p> <p>On what basis were the modeling results used?</p> <p>The magnitude of uncertainties associated with the modeling results will have an important bearing on the utility of <i>model applications</i>.</p>	<p>Modeller</p>
23	<p>What are the recommendations that follow from the modeling study?</p> <p><i>Explanation</i></p> <p>The recommendations that follow from the modeling study can be useful for future projects, for the design/adaptation of the monitoring programme and for model code improvement. Water manager, modeller and model code developer can profit Additional guidance from the recommendations.</p>	
	Considerations	

	Water Manager Consider an extra effort on monitoring: to reduce the uncertainties in the input data, to increase the dataset for <i>calibration/validation</i> and to cover all possible circumstances	Modeller Consider the technical flaws in the software. Consider the pitfalls in the application of the model code.
	Additional guidance	
	Water Manager Share your experiences with other water managers.	Modeller Inform the model code developer about the recommendations for model code improvement. Share your experiences with other modellers.
	Additional guidance	
	Water Manager Decisions are made on the basis of many more sources of information than model results only. Does new monitoring data (if any) show accordance with simulated effects of measures?	Modeller

N.B.: The Model Evaluation Tool (MET) is designed to facilitate choice of a suitable model code for application in the context of a management task or range of tasks. The selection process may not lead to an optimal choice of model code suitable for all associated tasks. Successful application can never be guaranteed. Neither the authors, nor other participants within the BMW consortium accept responsibility if unsatisfactory model applications arise following use of the benchmarking MET.

Table A1.4: Summary on selected catchment water quality models (acronyms in the table is listed in A1.5)

Models Model components		Empirical model		Conceptual model			Physically –based model		
		AGNPS	CNS	SWAT	HSPF	HBV	ANSWERS-2000	SHE and SHETRAN	DWSM
Hydrology	Evaporation/ evapotranspiration	No	Potential evapotranspiration (PET) using Hamon equation (Hamon 1961, cited in Haith et al., 1984))	For both potential and actual evapotranspiration with different algorithms e.g. Penman-Monteith method	Evapotranspiration and potential evaporation (PE) (eg.Penman formula for PE, Jensen formula for PET)	Potential evapotranspiration is used as input data (usually calculated based on the Penman formula)	Actual evapotranspiration model using Ritchie’s method (Ritchie, 1972, cited in Bouraoui and Dillaha, 1996)	Actual evapotranspiration model using Penman-Monteith equation	No
	Interception, surface storages	SCS CN method	SCS CN method	SCS CN method as well as the maximum storage in canopy calculated using Leaf area index (LAI)	Water balance equation	Water balance equation	Water balance equation	Dynamic change storage using modified Rutter model (Rutter et al., 1971/72. cited in Abbott et al., 1986)	Canopy interception, ground-cover interception and depression storage
	Runoff generation	Runoff volume using runoff SCS CN	Modify SCS CN method plus soil moisture for continuous simulation	Adjustment of SCS CN method for continuous simulation (improving solutions for soil moisture, slope)	Surface runoff and interflow as a function with infiltration capacity	Runoff generation is transformed excess water from the soil moisture zone to runoff using response function	Runoff generated when rainfall excess infiltration capacity and surface retention	Water balance equation (rainfall minus evaporation, evapotranspiration, interception and infiltration)	Runoff SCS CN
	Infiltration	Included in the SCS CN	Water balance equation	Green & Ampt equation	Empirical formula	Embedded in soil moisture accounting	Green & Ampt equation	1-D Recharts equation	Water balance and 1-D diffusion equation of water under gravity
	Percolation into ground water	No	Water balance equation	Empirical formula	Empirical formula	Constant parameter	Based on Brooks and Corey equation (1964, cited in Bouraoui et al., 2002)	1-D Recharts equation	No
	Overland flow routing	Flow peak using an empirical relation as in CREAMS model or TR55 method as triangular – shaped channel	Total storm runoff is estimated as a trapezoid-shape including peak and time of concentration, storm duration	Flow peak using modified rational formula and time of flow concentration is calculated by empirical formula	Chezy-Manning equation	Muskingum method or simple time lags	Continuity equation with stage – discharge relationship	2-D diffusive wave equations	1-D kinematic wave equations
	Groundwater flow	No	No	Using kinematic storage model (including transmission loss)	Using recession model	Using recession model	Interflow and groundwater flow (unsaturated zone) simulated using Darcy equations	Boussinesq equation as combined Darcy’s law and mass conservation of 2-D laminar flow	Kinematic storage model

<div>Models</div> <div>Model components</div>		Empirical model		Conceptual model			Physically –based model		
		AGNPS	CNS	SWAT	HSPF	HBV	ANSWERS-2000	SHE and SHETRAN	DWSM
	Reservoir	Flow, sediment and contaminants routing through impoundment terrace system having pipe outlet	No	Flow routing using water balance equation and sediment/contaminant routing using mass balance equation	Using kinematic wave or storage-routing method. sediment/contaminant routing using CSRT model	Flow routing using water balance (storage- discharge relation) and sediment/contaminant routing using mass balance equation	No	No	Storage indication (SCS, 1972, cited in Borah et al., 2002) or Puls method
Erosion and sedimentation	Detachment by rain	Included in the modified USLE formula	No	No	Rainfall splash detachment using empirical equation	No information (GIS-based operation)	Called as interrill erosion derived based on the USLE parameters	Rain drop and leaf drip modelled using empirical equation	Empirical equation (Mutchler and Young, 1975, cited in Borah et al., 2002)
	Detachment by flow	Included in the Modified USLE formula	Included in the Modified USLE formula	Included in the Modified USLE formula	Wash off for scour using empirical equation	No information (GIS-based operation)	Called as rill erosion using the modified USLE equation	Called sheet flow using empirical equation	Scours calculated based on potential exchange rate (embedded in continuity equation for sediment routing)
	Transport capacity	Bagnold steam power equation	No	No	Using empirical equation	No information (GIS-based operation)	Using the modified Yalin equation	Using the modified Yalin equation or Hagelund-Hansen equation	Using Yalin equation for overland; Yang and Laursen formulas for channel
	Sediment composition	Five classes (Foster et al., 1985)	Five classes (Foster et al., 1985)	No	Three classes (sand, silt, clay)	No information	Ten classes	Varies with sediment sizes and types	5 classes (Foster et al., 1985)
	Deposition on overland surface	Calculated when sediment load excess transport capacity (e.g. in WEPP model)	No	No (only in stream sediment routing)	No	No information	Yes, to describe settling efficiency	As differences between available sediment and transport capacity	Based on potential exchange rate (embedded in continuity equation for sediment routing)
	Gully erosion	As input	No	No	As scour using empirical equation	No information	No	No	No
	Overland sediment routing	Steady-state continuity equation	No	Accumulated in the main channel by relating to runoff time lag and time lag of concentration for HRUs	Lumped for each time step using power equation	No information	Continuity equation	2-D advection – dispersion equation	Sediment continuity equation
	Applied fertilizer	As input	As input	N and P in organic and inorganic forms as input	No (only as available mass/ concentration)	As input	No (only as available mass/ concentration)	Can be added as sources into advection-dispersion equation	Can be added as sources in mass balance equation
	Atmospheric	As input	As input	As input	As concentration	As input	No	Can be added as	Can be added as

Models Model components		Empirical model		Conceptual model			Physically –based model		
		AGNPS	CNS	SWAT	HSPF	HBV	ANSWERS-2000	SHE and SHETRAN	DWSM
Nutrient	deposition				input (later calculated as mass)			sources into advection-dispersion equation	sources in mass balance equation
	Point sources	As input	No	As external sources	Yes (as daily loads)	As input	No	Can be added as sources into advection-dispersion equation	
	Separated forms	Soluble and sediment associated for nitrogen and phosphorus	In solid-phase and dissolved forms for both nitrogen and phosphorus	In various from of nitrogen and phosphors (organic, inorganic, soluble, adsorbed)	In various from of nitrogen and phosphors (organic, inorganic, soluble, adsorbed)	Coupling with SOIL-N model (in various forms)	In various from of nitrogen and phosphors (organic, inorganic, soluble, adsorbed)	In solid-phase and dissolved forms	Dissolved and adsorbed chemicals
	Nutrient transformation in soil	No	Neglecting denitrification	Represent nitrogen and phosphorus cycle in soil	Represent nitrogen and phosphorus cycle in soil	Coupling with SOIL-Nor ICECREAM model) (in various forms)	Represent nitrogen and phosphorus cycle in soil	Partly i.e. plant uptake using Michaelis-Menten equation; adsorption using Freudlich equation; radioactive decay based on half-life of the contaminants ; absorption in dead-space (immobile water)	Only adsorption and desorption
	Nutrient transport in runoff and eroded sediment	Calculation of soluble nitrogen and phosphorous in runoff using extraction coefficients, while sediment attached contaminant calculated based on enrichment ratios	Dissolved nutrient calculated based on concentration in top centimetres soil and fraction of available runoff ; while adsorbed nutrient calculated based on enrichment ratio	Calculation of Nitrate-N based on water volume and average concentration, Dissolved P based on partitioning factor; organic N and sediment adsorbed P losses using loading functions based on enrichment ratios. Accumulated in the main channel by using runoff time lag and time lag of concentration for HRUs	Using empirical equation	Dynamic mass-balance model	Sediment-bound nutrient simulated based on conservation of mass as in Storm et al (1988, cited in Bouraoui et al., 2002); Dissolved nutrient is based on mass balance approach using extraction coefficient with partition coefficients	1-D advection – dispersion equation	1-D mass balance equation
	Leaching and transported by groundwater	No	Percolation loss of nitrogen as function of fraction of available water and	For both nitrogen and phosphorus based on percolation coefficient	Using empirical equation	Coupling with SOIL-N or ICECREAM model	Nitrate is leached through infiltration and percolation based on mass	3-D advection – dispersion equation	Using mass balance equation with partition coefficient

Models Model components		Empirical model		Conceptual model			Physically –based model		
		AGNPS	CNS	SWAT	HSPF	HBV	ANSWERS-2000	SHE and SHETRAN	DWSM
			concentration				balance approach with extraction coefficient of 0.5		
River routing	Hydraulic/hydrologic routing	Included in overland flow routing	No	Routing based on variable storage coefficient method and flow using Manning's equation adjusted for transmission losses, evaporation, diversions, and return flow.	Using kinematic wave or storage-routing method	Transfer function or Muskingum routing	Continuity equation with Manning stage – discharge relationship	1-D diffusive wave equations	Kinematic wave equation
	Sediment routing (including sources/sinks)	Included in overland sediment routing	No	Simplified the Bagnold stream power equation as well as including channel erodibility factor, sediment deposition	Non-cohesive (sand) sediment transport using user-defined relation with flow velocity or Toffaleti Colby method, or power function; cohesive (silt, clay) based shear stress calculation	Dynamic mass-balance model	Included in overland sediment routing	1-D advection – dispersion equation including erosion, deposition	Mass balance equation for sediment (including streambed scour)
	Nutrient routing (including sources/sinks, transformations)	Included in overland flow/sediment routing (no transformation processes involved)	No	Modify mass transport equation including advection, dispersion, dilution, interactions; Source and sink components in the QUAL2E model	Advection, deposition and scour (CSTR model)	Dynamic mass-balance model	Included in overland sediment routing	1-D advection – dispersion equation (simple in transformation i.e. adsorption, radioactive decay, erosion, deposition)	Mass balance equation for chemicals
Spatial discretization		Uniform square areas (cells), some containing channels /impoundment. 1-D simulation. Few arcs – 50,000 arcs	Lumped as 1 modeling unit (field scale as several hectare)	Sub-basins grouped based on climate as Hydrologic Response Units – HRU (lumped similar cover, soil, and management areas), ponds, groundwater, and main channel. 1-D simulation.	Land use discretization as lumped modeling units (including fraction of pervious and impervious), Stream channels, and mixed reservoirs simulated separately; 1-D simulations. From small	Each sub catchment as a modeling unit (from 1 km ² to > 1,000,000 km ²)	Discretized into square cells with uniform hydrologic characteristic (max. 1ha) some having companion channel elements. 1-D simulation. Ranging from field scale (few hectares) to small catchment	2-D rectangular/ square overland grids, 1-D channels, 1-D unsaturated and 3-D saturated flow layers. Ranging from field scale (few hectares) to river basin (hundred, thousand km ²)	Overland, channel, and reservoir segments defined by topographic –based natural boundaries; 1-D simulations Field scale (few ha) to medium catchment (hundred km ²)

<div>Models</div> <div>Model components</div>		Empirical model		Conceptual model			Physically –based model		
		AGNPS	CNS	SWAT	HSPF	HBV	ANSWERS-2000	SHE and SHETRAN	DWSM
				From few km ² (e.g. 0.5) thousand km ² (e.g. 80,256)	catchment to river basin scale		(few km ²)		
Temporal discretization		Storm event; one step is the storm duration	A daily time step for hydrologic processes and a monthly time step for chemical balances	Long term; daily time steps. Hourly time steps implemented in ESWAT model (Van Griensven and Bauwens, 2001)	Long term hourly/daily time steps	Long term; daily time steps.	Long term , daily time steps	Long term and storm event; variable steps depending numerical stability	Storm event; variable constant steps
User interface		No, but adapted to other model e.g. WaSiM-ETH, GRIPs	No	In GRASS, AVSWAT for ARCVIEW, ArcSWAT for ARCGIS, Map-Window SWAT	Embedded in BASINS system also in independent WinHSPF	IHMS SYSTEM	Arcview interface	No, except SHE embedded in the commercial packet MIKE-SHE	No
Uncertainty analysis (examples)		MCMC (Balin et al., 2008); Monte-Carlo, DYNIA (Wriedt and Rode, 2006)	Calibration is not needed!	Automated sensitivity analysis, calibration and input uncertainty analysis (Van Griensven and Bauwens, 2003)	Evolutionary Algorithm (Castanedo et al., 2006); FOA, Monte-Carlo (Wu et al., 2006)	Monte-Carlo (Harlin and Kung, 1992; Seibert, 1997)	Monte-Carlo (De Roo et al., 1992)	GLUE method (e.g. in Ewen et al., 2007)	No information
References		(Young et al., 1995; Young et al., 1989)	(Haith and Tubbs, 1981; Haith et al., 1984)	(Arnold and Fohrer, 2005; Gassman et al., 2007; Neitsch et al., 2005)	(Bicknell et al., 2001)	(Arheimer, 2003; Arheimer and Brandt, 2000; Bergstrom, 1995)	(Beasley et al., 1980; Bouraoui et al., 2002; Bouraoui and Dillaha, 2000)	(Abbott et al., 1986; Ewen, 1995; Ewen et al., 2000; Lukey et al., 1995)	(Borah et al., 2003; Borah et al., 2002)
Remarks								Groundwater exchange also simulated	

(*) Parts of this table were adapted from Borah and Bera (2003)

Table A1.5: Acronyms for model names and others

Acronyms	Full version
AGNPS	<u>A</u> gricultural <u>N</u> on- <u>P</u> oint <u>S</u> ources
CNS	<u>C</u> ornell <u>S</u> imulation <u>m</u> odel
SWAT	<u>S</u> oil and <u>W</u> ater <u>A</u> ssessment <u>T</u> ool
HSPF	<u>H</u> ydrological <u>S</u> imulation <u>P</u> rogram - <u>F</u> ortran
GLEAMS	<u>G</u> roundwater <u>L</u> oading <u>E</u> ffects of <u>A</u> gricultural <u>M</u> anagement <u>S</u> ystem
HBV	<u>H</u> ydrologiska <u>B</u> yråns <u>V</u> attenbalansavdelning
MONERIS	<u>M</u> odeling <u>N</u> utrient <u>E</u> mission in <u>R</u> iver <u>S</u> ystems)
ANSWERS	<u>A</u> real <u>N</u> onpoint <u>S</u> ource <u>C</u> atchment <u>E</u> nvironmental <u>R</u> esponse <u>S</u> imulation
SHE	<u>S</u> ystème <u>H</u> ydrologique <u>E</u> uropéen
DWSM	<u>D</u> ynamic <u>C</u> atchment <u>S</u> imulation <u>M</u> odel
SCS CN	<u>S</u> oil <u>C</u> onservation <u>S</u> ervice <u>C</u> urve <u>N</u> umber (see Ogrosky and Mockus, 1964)
CREAMS	<u>C</u> hemicals, <u>R</u> unoff, and <u>E</u> rosion from <u>A</u> gricultural <u>M</u> anagement <u>S</u> ystems (Knisel and Walter, 1980)
WEPP	<u>W</u> ater <u>E</u> rosion <u>P</u> rediction <u>P</u> roject (Foster et al., 1995)
WaSiM-ETH	<u>W</u> ater balance <u>S</u> imulation <u>M</u> odel <u>E</u> idgenössische <u>T</u> echnische <u>H</u> ochschule (Schulla 1997)
GRIPs	<u>G</u> eo <u>R</u> eferenced <u>I</u> nterface <u>P</u> ackage for the Agnps 5.0 catchment model : geospatial interface software package between ILWIS V. 3.2 and the AGNPS v.5.0 (Mannaerts et al., 2002)
QUAL2	Enhanced Stream Water Quality Model (Brown and Barnwell, 1987)
ESWAT	<u>E</u> xtended <u>S</u> oil and <u>W</u> ater <u>A</u> ssessment <u>T</u> ool (Van Griensven and Bauwens, 2001) <u>E</u> nhanced <u>S</u> oil and <u>W</u> ater <u>A</u> ssessment <u>T</u> ool (Debele et al., 2008)
USLE	<u>U</u> niversal <u>S</u> oil <u>L</u> oss <u>E</u> quation
CSRT	<u>C</u> ontinuous- <u>S</u> tirred <u>T</u> ank <u>R</u> eactor
PET	<u>P</u> otential <u>E</u> vapotranspiration
PE	<u>P</u> otential <u>E</u> vaporation

2. Appendix 2: Surveyed areas



Figure A2.1: Sugar apple



Figure A2.2: Rubber



Figure A2.3: Rice field



Figure A2.4: Cassavas



Figure A2.5: Interviewing farmers



Figure A2.6: Using handheld positioning equipment



Figure A2.7: Organic fertilizers



Figure A2.8: Concrete irrigation canals



Figure A2.9: Rocky mountain (Nui Ba Den)



Figure A2.10: Rocky mountain (Nui Ba Den), closer view.



Figure A2.11: water sampling in upper stream.



Figure A2.12: Soil sampling: equipment (left), at cassava field (upper right), 8 samples at each land-use site (lower right)



Figure A2.13: Tra Phi bridge (measurement station was appr. 300m down stream of Tra Phi bridge)



Figure A2.13: Equipments at measurement station (ADCP, water level staff, instance water quality measurement for TDS, pH, DO, temperature)



Figure A2.14: Operating ADCP equipment (Flow discharge measurement), collecting flow data via



Figure A2.15: Photometer (Spectroquant NOVA 60)



Figure A2.16: Analysis of nutrient parameters (P-PO₄, N-NH₄, N-NO₃) using photometer



Figure A2.17: Setting-up measurement station



Figure A2.18: Manual water sampling



Figure A2.19: Wastewater discharge at tapioca company



Figure A2.20: Estimation of average wastewater flow velocity



Figure A2.21: Structure for estimation of average wastewater discharge



Figure A2.22: Figure Meteorological station



Figure A2. 23: Example of an Acrisol soil profile in Vietnam (Hapli Plinthic Acrisols) (Nguyen et al., 2006)

Table A2.2: Description of Acrisol soil profile in figure A2.23 (Nguyen et al., 2006)

Depth	Description
0-19 cm	Dull yellowish brown 10 YR 5/4 (wet), dull yellow orange 10YR 6/3 (dry); wet; few fine mottling, size < 6 mm, faint contrast; light loam; fine granular structure; not firm; high porosity; clear horizon boundary.
19-29 cm	Dull yellow orange 10 YR 6/3 (wet), dull yellow orange 10 YR 7/4 (dry); wet; few fine mottling, size < 6 mm, faint contrast; light loam; fine granular structure; not firm; high porosity; clear horizon boundary.
29-80 cm	Light yellow orange 10 YR 8/3 (wet), reddish brown 10 R 5/4 (dry); wet; abundant mottling, medium size from 6 to 20 mm, prominent contrast; loamy clay; medium blocky structure; firm; very low porosity; few residual rock fragment medium rounded nodules.

Table A2.2: Analysis of Acrisol soil profiles in figure A2.23 (Nguyen et al., 2006)

Depth (cm)	% of particle fraction				Total, %			Available mg/100 g of soil		
	Sand	Silt	Clay	OC	N	P ₂ O ₅	K ₂ O	N	P ₂ O ₅	K ₂ O
0-17	35.5	57.7	6.8	0.86	0.09	0.04	0.25	2.80	4.12	3.37
17-26	23.5	58.5	18.1	0.57	0.05	0.02	0.20	1.96	1.03	0.62
26-80	21.5	35.7	42.8	0.12	0.04	0.01	0.86	0.56	0.44	2.61

3. Appendix 3: Sample data

Table A3.1: Upstream sample data

Sample name	Time	DO	N-NO ₃ mg/l	N-NH ₄ mg/l	P-PO ₄ mg/l	TSS mg/l
27 Jul. 2008						
TPTN01	6.25	4.32	-	0.274	0.56	220
TPTN02	6.35	3.47	0.6	0.381	0.43	86
During event						
Rainfall	25/7/2008		<<	0.315	0.05	
5 Sep.2008						
TPT 1a	17:00	-	1.7	0.203	0.34	-
TPT 1b	17:00	-	1.1	0.196	0.4	116
TPT 2a	18:00	-	1.8	0.34	0.37	265
TPT 2b	18:00	-	0.9	0.353	0.75	490
6 Sep. 2008						
TPT 5a	11:00	-	<<	0.199	0.49	185
TPT 5b	11:00	-	1		0.58	160

<<: Smaller than identification limits

Table A3.2: Soil data

Samples	Land use	pH-H2	Chlorine mg/g	Humidity %	P-PO ₄ mg/kg	Total P mg/kg	NH ₃ mg/kg	Total N mg/l
1.	Sugar Apple	5.77	29	5	165	240	16.5	880
2.	Cassava	5.66	29	10.2	37	200	3.1	720
3.	Rubber	4.55	24	7.4	70	240	2.9	380
4.	Rice 1	5.71	29	13.2	117	260	14.5	310
5.	Sugar -cane	4.49	20	10.3	210	210	4.1	440
6.	Rice 2	5.86	29	3.4	26	190	16.5	610

Table A3.3: Water quality data at measurement station (Event 1, 25th July 2008 – 27th July 2008)

Sample name	Time	DO mg/l	TDS mg/l	To °C	pH	N-NO ₃ mg/l	N-NH ₄ mg/l	P-PO ₄ mg/l	TSS mg/l
25 Jul.2008									
TP01	16.00	1.35	27	31	5.84	-	0.062	0.35	592
TP02	18.00	1.89	25	28.7	5.91	0.5	0.135	0.43	684
19.00									
TP03	20.00	2.04	23	27.8	5.46	2.4	0.487	0.85	1085
TP04	22.00	2.74	27	27.3	4.96	1.9	0.459	0.84	1340
23.00									
26 Jul.2008									
TP05	00.00	2.59	31	27.4	5.24	0.8	0.652	0.82	404
1.00									
TP06	2.00	2.45	31	27.4	5.37	1	0.492	0.81	330
3.00									
4.00									
TP07	5.00	1.94	33	27	5.2	1.1	0.467	0.69	233
6.00									
TP08	7.00	2.02	34	27	5.41	1	0.361	0.69	252
8.00									
TP09	9.00	2.08	33	27.7	5.4	1.1	0.296	0.76	188
10.00									
TP10	11.00	2.45	33	29.3	5.45	0.6	0.319	0.96	218
TP11	13.00	1.87	35	31	5.47	1.4	0.408	0.9	208
TP12	17.00	1.44	36	30	5.21	1.3	0.147	0.65	86
18.00									
TP13	19.00	1.41	34	30	5.26	0.4	0.105	0.54	144
TP14	21.00	1.47	35	29.1	4.97	1.1	0.142	0.71	218
TP15	23.00	1.68	35	28.7	5.32	0.6	0.129	0.66	192
27 Jul.2008									
TP16	3.00	1.44	35	28.1	5.32	0.4	0.159	0.55	129
TP17	6.00	1.28	36	27.9	5.22	1	0.157	0.58	115

Table A3.4: Water quality data at measurement station (Event 2, 6th August 2008 – 8th August 2008)

Sample name	Time	DO mg/l	TDS mg/l	To °C	pH	N-NO ₃ mg/l	N-NH ₄ mg/l	P-PO ₄ mg/l	TSS mg/l
6 Aug. 2008									
TPL01	16.00	1.46	25	30	5.92	-	-	-	195
TPL02	18.00	1.23	24	28.8	5.8	-	-	-	129
7 Aug. 2008									
TPL03	17:00	1.5	24	28.8	5.96	0.4	0.125	0.25	130
8 Aug. 2008									
TPL04	6:00	2.3	102		4.7	0.7	2.302	3.65	186
TPL05	7:00	1.96	101	27	4.51	1	2.225	3.56	264
TPL06	9:00	2.08	81	27.2	4.78	1.2	1.849	2.54	208
TPL07	11:00	2.28	78	28.2	4.79	0.8	1.73	2.4	220
TPL08	15:00	-	80	28.4	4.8	0.3	1.642	2.62	150
TPL09	18:00	-	84	29.1	4.69	0.9	1.669	2.59	102
TPL10	20:00	-	76	28.2	4.79	0.4	1.75	2.56	152
TPL11	24:00	-	74	27.5	4.84	0.5	1.597	2.31	154
9 Aug. 2008									
TPL12	6:00	-	43	27.1	5.03	0.5	0.747	1.07	91

Table A3.5: Water quality data at measurement station (Event 3, 14th August 2008 – 15th August 2008)

Sample name	Time	N-NO ₃ mg/l	N-NH ₄ mg/l	P-PO ₄ mg/l	TSS mg/l
14 Aug. 2008					
TP05	10:30	0.4	0.183	0.43	58
TP06	17:30	0.6	0.473	0.63	490
TP07	18:30	1	1.378	1.08	1988
TP08	19:30	1.1	0.431	1.01	940
TP09	20:30	1	0.256	0.82	582
TP10	22:30	0.9	0.194	0.61	377
15 Aug. 2008					
TP11	0:30	1	0.536	0.93	310
TP12	2:45	1.2	0.398	0.81	213
TP13	5:00	1.1	0.395	0.83	149
TP14	7:00	0.7	0.793	0.91	153
TP15	9:00	0.6	0.718	0.84	122

Table A3.6: Data for setting up the Stage-Discharge curve

Number of measurement	H (m)	Q (m ³ /s)
1	0.18	1.66
2	0.34	2.33
3	0.40	2.63
4	0.53	3.26
5	0.70	4.32
6	0.74	4.57
7	0.70	4.14
8	0.68	3.98
9	0.66	3.72
10	0.65	3.62
11	0.64	3.56
12	0.63	3.42
13	0.59	3.16
14	0.52	2.84
15	0.45	2.46
16	0.00	1.13
17	0.00	1.23
18	0.00	1.20
19	0.00	1.13
20	0.00	1.24
21	0.60	3.18
22	0.50	2.76
23	0.48	2.53
24	0.41	2.37
25	0.40	2.28
26	0.43	2.49
27	0.48	2.80

4. Appendix 4: Additional information of the HSPF model

4.1. Model representations

4.1.1. Model discretization

In HSPF, a catchment is discretized into sub-catchment by means of GIS (implemented in BASIN system). Simulated variables (e.g. runoff, water quality constituents) are accumulated at each sub-catchment outlet and then are routed through river reaches or reservoirs called RCHRES. Inside each sub-catchment, land-uses are modeling units where physical processes/characteristics are uniformly distributed in within each land use (lumped); No interaction (storages and fluxes) among different land use types (e.g. see in Figure A4.1) because the water balance on each PLS is calculated independently and is routed to the nearest stream. The land-use is considered as pervious or/and impervious in term of percentage (see Figure A4.2). This will be later considered for modeling purposes. Those processes occurred in pervious areas are modelled by PERLND module, while those in impervious ones are simulated by IMPLND module. The PERLND, IMPLND and RCHRES are described in the following section.

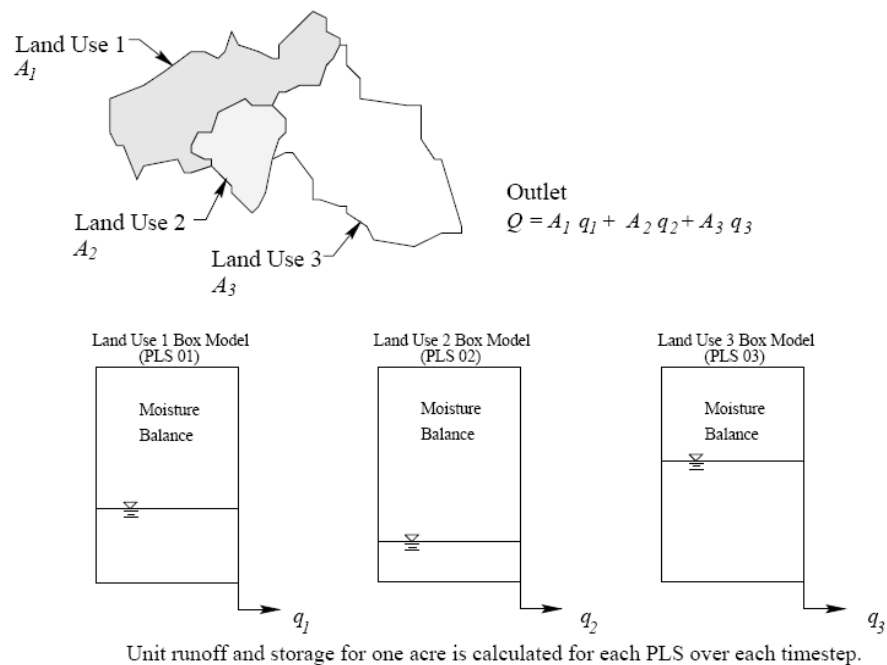


Figure A4.1: Schematic of the land use discretization in HSPF showing the independence of the individual PLSs and the calculation of the simulated catchment runoff from the unit runoff each PLS (Socolofsky, 2002)

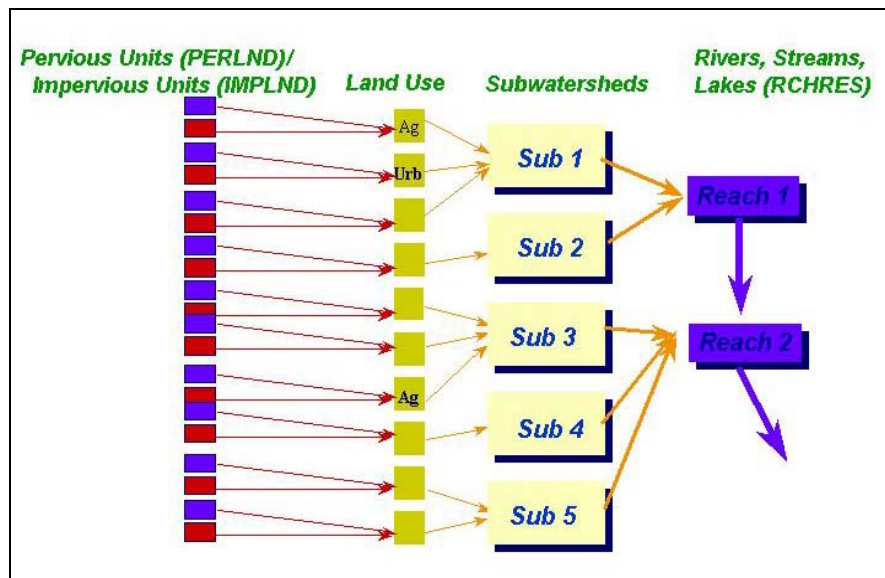


Figure A4.2: Model Segmentation in HSPF (Tetra Tech, 2004)

4.1.1.1. PERLND

PERLND simulates water quality and quantity processes occurring on a pervious areas (Bicknell et al., 2001; Donigian et al., 1995). Different processes are modelled through a number of components and are illustrated in Figure A4.3. The main processes and implemented sub-modules (in bracket) are as follows:

- Snow accumulation and melt (SNOW)
- Water budget (PWATER)
- Erosion and sedimentation (SEDMNT)
- Water quality constituents (PQUAL, MSTLAY, PEST, NITR, PHOS, TRACER) where “PQUAL” is applied based on simple relationship when soil data is limited; “MSTLAY” simulates solute transport; “PEST” simulates pesticides; “NITR” and “PHOS” simulates nitrogen and phosphorus compositions, respectively; “TRACER” simulates conservative tracer.
- Air, soil temperature (ATEMP, PSTEMP, respectively)
- Water temperature and gas concentrations (PWTGAS)

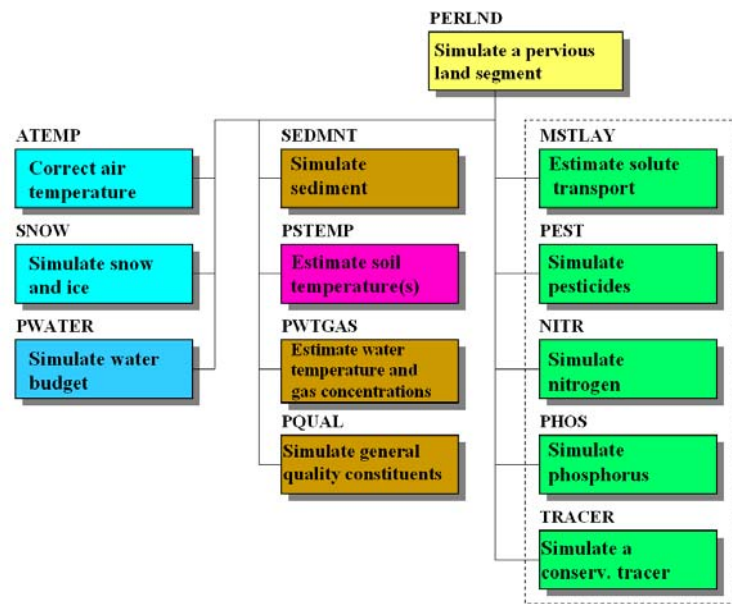


Figure A4.3: PERLND structure chart (US EPA, 2009)

4.1.1.2. IMPLND

Similarly (to the PERLND module), the IMPLND module simulates water quality and quantity processes occurring on a impervious areas, however, processes occurring in here are less than the pervious areas. For example, erosion caused by soil detachment or infiltration does not occur. The main processes are as follows and are shown in Figure A4.4

- Water budget (IWATER)
- Erosion and sediment (SOLIDS)
- Water temperature and gas concentrations (IWTGAS)
- Water quality constituents (IQUAL) based on simple relationship
- SNOW and ATEMP in PERLND are shared with IMPLND since they can be applied to pervious or impervious segments.

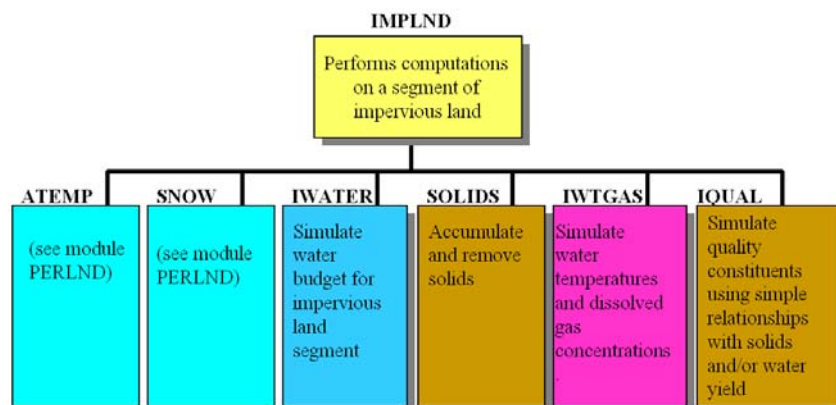


Figure 4.4: IMPLND structure chart (US EPA, 2009)

4.1.1.3. RCHRES

The RCHRES can be used to model behaviour of water quantity and water quality processes through stream and reservoir. The main processes simulated in RCHRES module are clearly identified in figure A4.5 including: hydraulic behaviour (HYDR), advective behaviour of constituents (ADCALC), conservative constituents (CONS), heat exchange and water temperature (HTRCH), inorganic sediment (SEDTRN), biochemical transformation of constituents (RQUAL) and generalized quality constituents e.g. through decay, volatilization, adsorption and desorption, advection of dissolved and suspended materials processes (GQUAL)

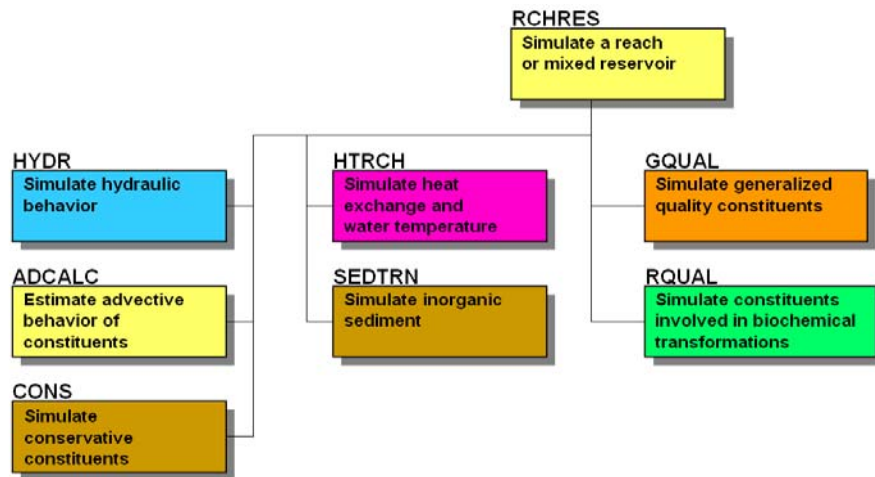


Figure A4.5: RCHRES structure chart (US EPA, 2009)

4.1.2. Modeling components

HSPF is a one of the most complex catchment water quality models. Model structure and model algorithms are, therefore, comprehensive. As presented in the previous section, different water quantity and water quality processes are simulated in the model. In term of nutrient modeling at catchment scale, typical processes involved are: hydrological processes; soil erosion and sediment transportation; nutrient transformation and transport; and river/reservoir routing. Most of the physical aspects of these processes are similar to those explained in chapter 2. Thus, in this section it is devoted to explain how these processes are modelled in HSPF model.

While the model utilizes a number of conventional algorithms (from other studies, e.g. Manning formula, Freundlich isotherm), some other algorithms were developed for the model itself (Bicknell et al., 2001; Radcliffe and Lin, 2007).

4.1.2.1. Hydrology components

The main hydrologic processes modelled in HSPF are shown in Figure A4.6 The governing hydrological equation is basically the water balance equation as follows

Water balance equation:

$$P + SWI + GWI = ET + SWO + GWO + \Delta S \quad (\text{eq. A4.1})$$

Where:

P = Precipitation
 SWI, SWO = surface water inflow, surface water outflow

GWI, GWO = groundwater inflow, groundwater outflow
 ET = Evapotranspiration
 ΔS = change in storage

From this equation, the most important processes are: infiltration, percolation, and lateral flow to river network (including overland flow, interflow, and groundwater flow) as presented in appendix 4 (section 1.2)

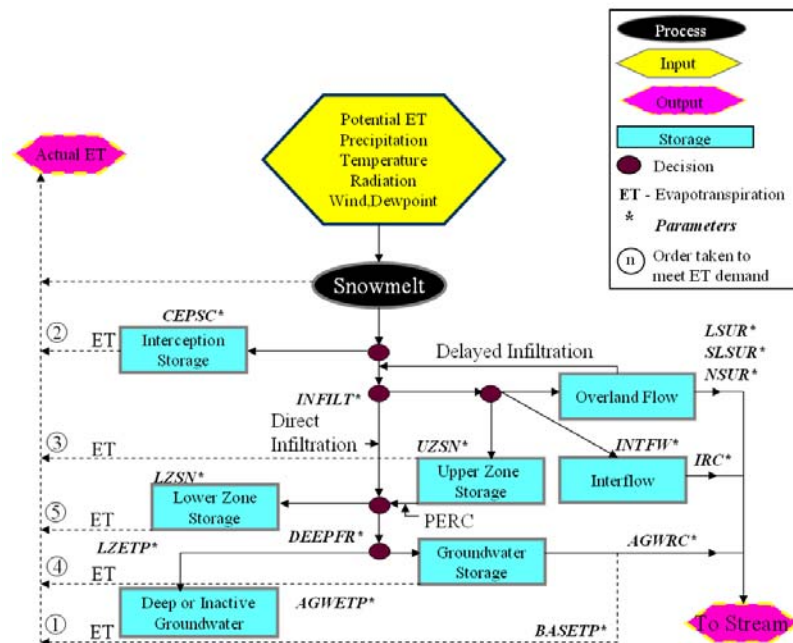


Figure A4.6: Hydrology processes in HSPF model (US EPA, 2009)

4.1.2.2. Erosion components

Erosion processes and sediment transportation are modelled in SEDMNT module. A flow diagram for SEDMNT module is shown in Figure A4.7. Basically, the calculation of eroded materials in the HSPF model follows some principles explained in chapter 2 e.g. calculation of the detachment, and transport capacity. The differences between these two are sediment transported downstream. As presented in section 4.1.1, land surfaces are classified into pervious and impervious segments. Thus, model approaches to erosion processes and sediment transportation for these segments are different. In pervious segments, included processes are: Accumulation, detachment, transport, scour; whereas in impervious areas, only accumulation and transport are simulated since detachment and scouring are assumed not being occurred.

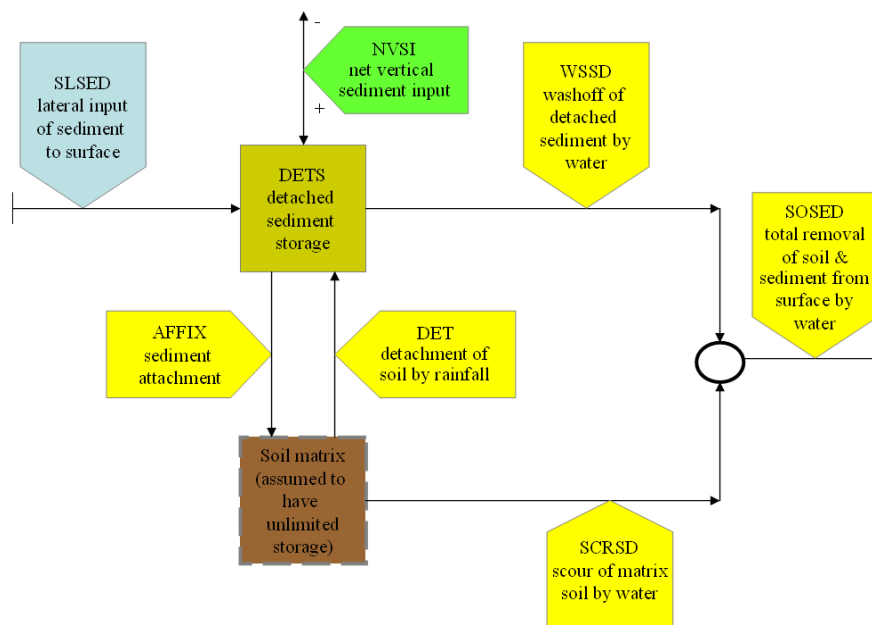


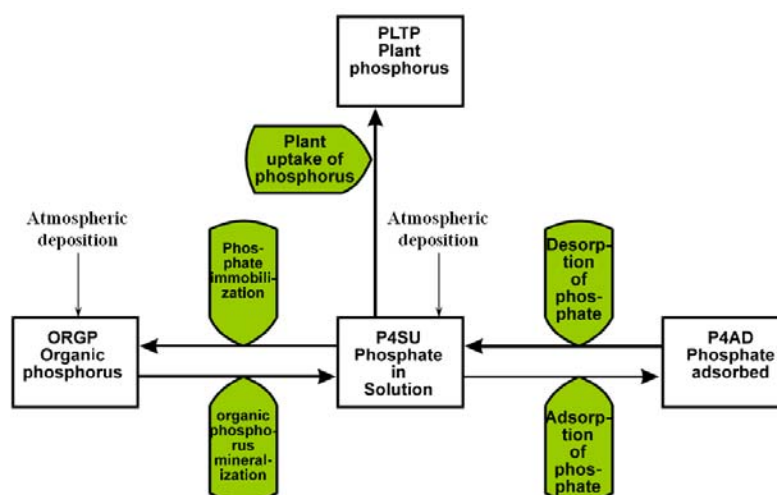
Figure A4.7: Flow diagram for SEDMNT module (US EPA, 2009)

4.1.2.3. Nutrient components

In the nutrient section, it is limited on only to inorganic nitrogen (N-NO_3 , N-NH_4) and inorganic phosphorus (P-PO_4) since these parameters are subjects to be modelled.

a. Nutrient transformation in soil

The main transformation processes of nutrient (nitrogen and phosphorus) in soil such as adsorption/desorption, plant uptake, immobilization, mineralization, denitrification, nitrification, volatilization that are modelled in HSPF are illustrated in Figure A4.8, Figure A4.9. Selected model algorithms are presented in appendix 4



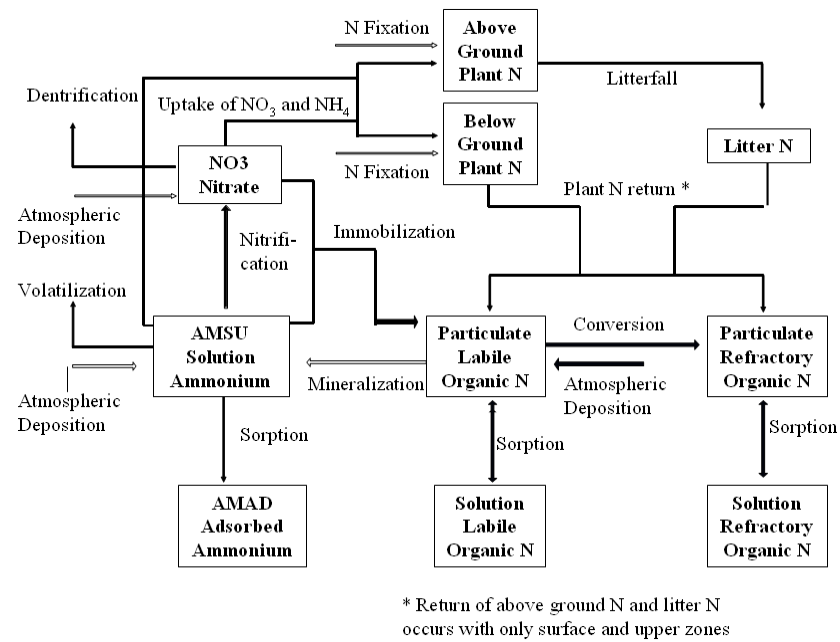
PLTP: Phosphorus stored in plants

P4SU: Solution phosphate

ORGP: Organic phosphorus

P4AD: Adsorbed phosphate

Figure A4.8: Nitrogen transformations simulated in HSPF (US EPA, 2009)

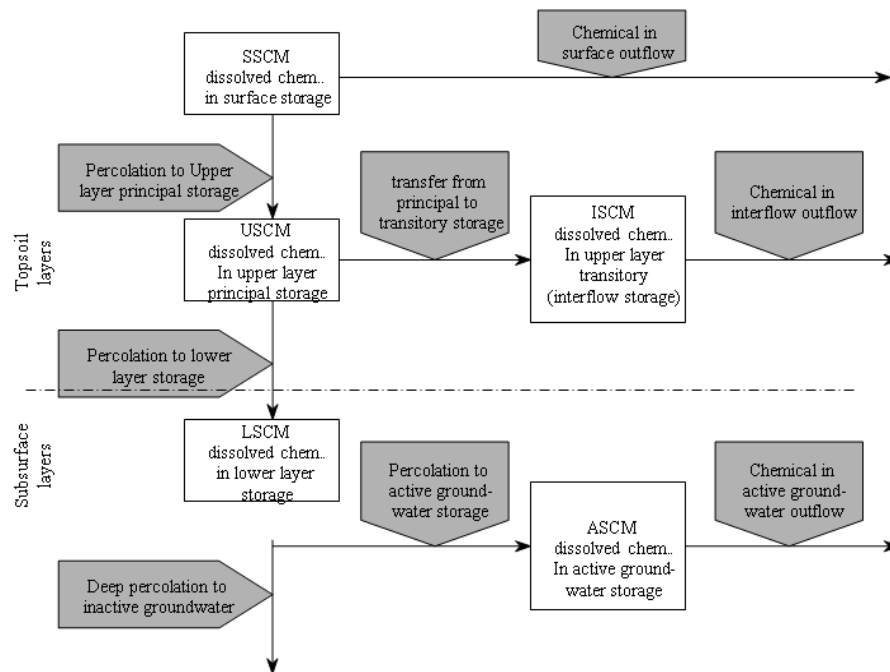


AMSU: Solution ammonium

AMAD: Adsorbed ammonium

Figure A4.9: Nitrogen transformations simulated in HSPF (US EPA, 2009)

b. Nutrient transport to river



SSCM: Dissolved chemical in surface storage

USCM: Dissolved chemical in upper layer storage

ISCAM: Dissolved chemical in upper layer transitory (interflow) storage

LSCM: Dissolved chemical in lower layer storage

ASCM: Dissolved chemical in active groundwater storage

Figure A4.10: Flow diagram for movement of solutes (US EPA, 2009)

Dissolved nutrient transport

The concentration of dissolved constituents is assumed the same as it is from the original storage (surface, upper ground water, ground water) and will contribute to stream as runoff, interflow and ground water flow and shown in Figure A4.10.

Particulate nutrient transport

In HSPF, the particular constituent removed from the land surface is assumed to be proportional to the solids removal. Thus, the removal of particulate nutrients (adsorbed ammonium and phosphate) and organic form of the nutrients by solids washoff are simulated by multiplying the eroded sediment (results from the erosion module) with a so-called wash-off potency factor. In addition, there are also direct wash-off constituents from the land surface which are accumulated previous. A schematic of associated-sediment nutrients is shown in Figure A4.11.

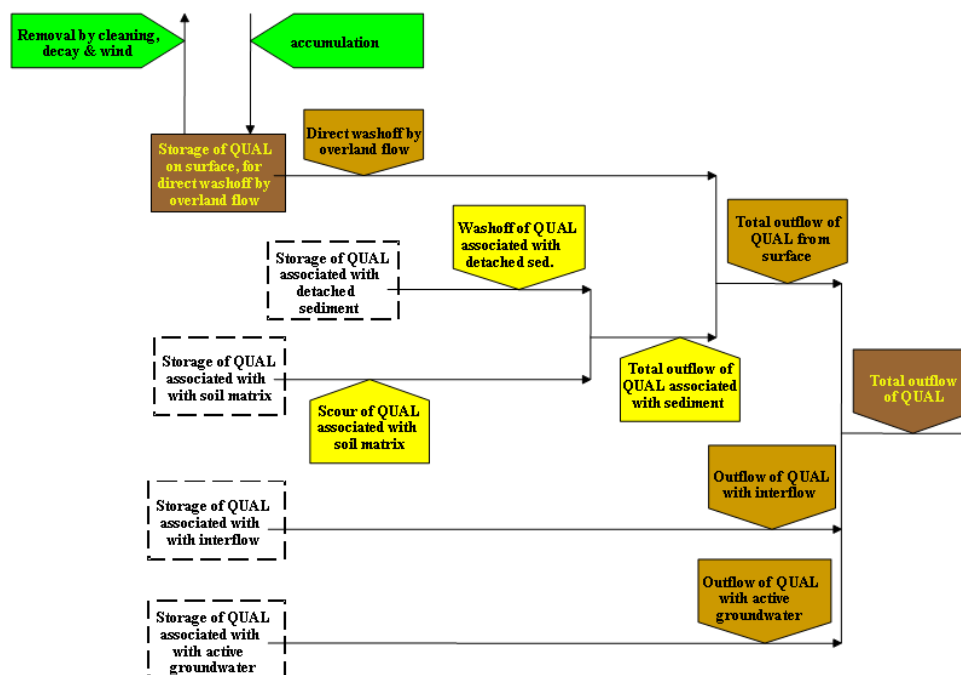


Figure A4.11: Pollutant accumulation and washoff in pervious areas (US EPA, 2009)

4.1.2.4. River routing

a. Flow routing

Flow routing in HSPF is modelled by kinematic wave or storage-routing method (i.e. conservation of momentum not considered). This is applied for unidirectional flow and considering river reach as completely mixed (single layer). In this way, it is required a function table (Ftable) for depth-area-volume-discharge relationship for each reach. A schematic of inflows to and outflows from a stream reach is presented in Figure A4.12.

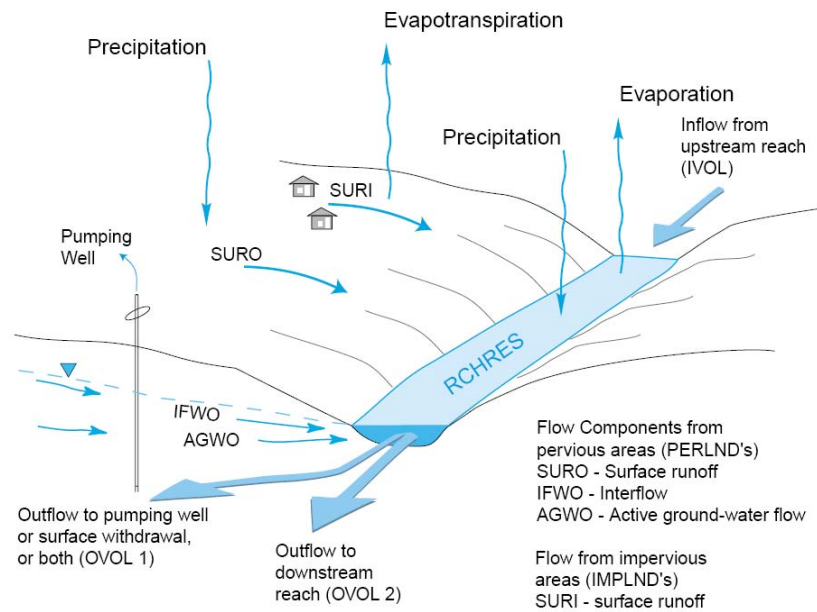


Figure A4.12: Schematic of inflows to and outflows from a stream reach (RCHRES) in the Hydrological Simulation Program-FORTRAN (HSPF). (Phillip and Kernell, 2000)

Water balance equation for each reach is:

$$VOLE = VOLS + \sum IVOL - \sum OVOL + PR - EVAP \quad (\text{eq. A4.2})$$

Where:

VOLE	=	volume at end of time step
VOLS	=	volume at start of time step
OVOL	=	outflow volumes (OVOL 1, OVOL2)
IVOL	=	inflow volumes (SURF, SURO, IFWO, AGWO)
PR	=	volume of precipitation
EVAP	=	volume of evaporation
\sum	=	Summation

The F Table can be generated based on GIS processing using some concept presented in Mohamoud and Parmar (2006) or can be measured from the field (i.e. the stage – discharge curve)

b. Sediment routing

SEDTRN section in RCHRES module simulate inorganic sediment load into three components which are sand, silt, and clay. Transport, deposition and scour of sand can be simulated by three different methods i.e. Toffaleti, method, and Power function, while silt and clay particles are calculated using the critical shear-stress theory.

c. Nutrient routing

A zero-dimensional well mixed box model was used in the river reach based on the following governing equation: (Tang, 1993)

$$\frac{dCV}{dt} = I_i + Q_o C + S \quad (\text{eq. A4.3})$$

Where:

- C = Constituent concentration in the box, mg/l (Kcal/m² in case of temperature computation)
- V = Volume of the water in the box, m³
- t = Time, sec
- I_i = Inflow mass flow rate of the constituent into the box, g/sec (Kcal-m/sec in case of temperature computation)
- Q_o = Water outflow rate from the box, m³/s
- S = Source/sink term for constituent concentration, mg/sec (Kcal-m/sec in case of temperature computation)

Advection, diffusion, transformation are the main mechanisms happening when contaminants reach to river networks. It is done through processes including hydrolysis, oxidation by free radical oxygen, photolysis, volatilization, biodegradation, and temperature dependent first-order decay (some processes are presented in appendix 4). Nutrient routing in HSPF is modelled using the continuous-stirred tank reactor (CSTR) as mentioned in chapter 2, section 2.5.3 “Contaminant river routing”.

4.2. Selected HSPF algorithms

4.2.1. Hydrology

Infiltration

The infiltration processes is unique for the HSPF model, as illustrated in Figure A4.13. This process relies on the calculation of the mean, maximum, minimum infiltration capacity (IBAR, IMAX, IMIN, respectively). Below the line 1 is the total area that infiltrates to the lower zone, whereas upper the line I is the area that contributes to direct runoff (overland flow, interflow, and detention on surface)

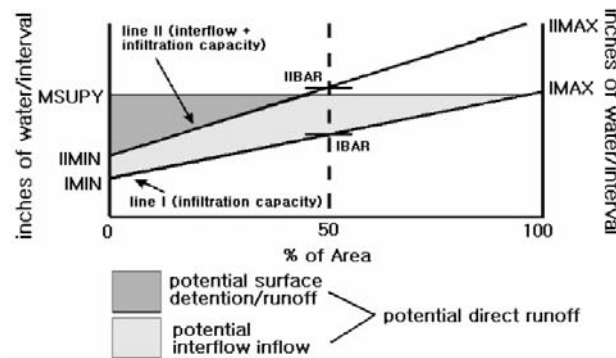


Figure A4.13: Determination of infiltration and interflow inflow (US EPA, 2009)

$$IBAR = \frac{INFIL}{\left(\frac{LZS}{LZSN}\right)^{INFEXP}} \times INFFAC \quad (\text{eq. A4.4})$$

$$IMAX = INFILD \times IBAR$$

$$IMIN = IBAR - (IMAX - IBAR)$$

$$RATIO = INFIW \times (2.0)^{\frac{LZS}{LZSN}}$$

Where:

IBAR	=	Mean infiltration capacity over the land segment (in/interval)
INFILT	=	Infiltration parameter (in/interval)
LZS	=	Lower zone storage (inches)
LZSN	=	Parameter for lower zone nominal storage (inches)
INFEXP	=	Exponent parameter greater than one
INFFAC	=	Factor to account for frozen ground effects, if applicable
IMAX	=	Maximum infiltration capacity (in/interval)
INFILD	=	Parameter giving the ratio of maximum to mean infiltration capacity over the land segment (recommended value of 2)
IMIN	=	Minimum infiltration capacity (in/interval)
RATIO	=	Ratio of the ordinates of line II to line I
INTFW	=	Interflow inflow parameter

Percolation

Water percolates from the upper zone to low zone storage. Percolation only occurs when UZRAT minus LZ RAT is greater than 0.01, and is calculated using an empirical formula as follows:

$$PERC = 0.1 \times INFILT \times INFFAC \times UZSN \times (UZ RAT - LZ RAT)^3 \quad (\text{eq. A4.5})$$

Where:

PERC	=	percolation from the upper zone (in/interval)
INFILT	=	infiltration parameter (in/interval)
INFFAC	=	factor to account for frozen ground, if any
UZSN	=	parameter for upper zone nominal storage (inches)
UZ RAT	=	ratio of upper zone storage to UZSN
LZ RAT	=	ratio of lower zone storage to lower zone nominal storage

Lateral flow contributions (surface, interflow, groundwater)

Overland flow

Overland flow is simulated using the Chezy-Manning equation and an empirical expression which relates outflow depth to detention storage. The rate of overland flow discharge is determined by the equations:

For SURSM < SURSE:

$$SURO = DELT60 \times SRC \times \left(SURSM \times \left(1.0 + 0.6 \times \left(\frac{SURSM}{SURSE} \right)^3 \right)^{1.67} \right) \quad (\text{eq. A4.6})$$

Or for SURSM > SURSE

$$SURO = DELT60 \times SRC \times (SURSM \times (1.6)^{1.67}) \quad (\text{eq. A4.7})$$

Where:

SURO	=	surface outflow (in/interval)
DELT60	=	DELT/60.0 (hr/interval)
SRC	=	routing variable, described below
SURSM	=	mean surface detention storage over the time interval (in)
SURSE	=	equilibrium surface detention storage (inches) for current supply rate

DELT = simulation time interval (min)

Interflow

The potential interflow is the area between line I, and line II in Figure A4.1. The interflow is estimated by:

$$IFWO = K2 \times IFWS + K1 \times INFLO \quad (\text{eq. A4.8})$$

Where:

IFWS = interflow storage at start of time step
 INFLO = addition to interflow storage during timestep
 IRC = Interflow recession parameter

K1, K2 are variables calculated by:

$$K1 = 1.0 - \frac{K2}{K}$$

$$K2 = 1.0 - e^K$$

$$K = -\ln(IRC) \frac{DELT60}{24}$$

This estimation is also unique of the HSPF model (Radcliffe and Lin, 2007)

Groundwater outflow

Contributed water to groundwater from infiltration and percolation can go to deeper groundwater storage or contribute to stream network as groundwater outflow that is estimated by:

$$AGWO = KGW \times (1.0 + KVAR \times GWVS) \times AGWS \quad (\text{eq. A4.9})$$

Where:

AGWO = active groundwater outflow (in/interval)
 KGW = groundwater outflow recession parameter (/interval)
 KVAR = parameter which can make active groundwater storage to outflow relation nonlinear (/inches)
 GWVS = index to groundwater slope (inches)
 AGWS = active groundwater storage at the start of the interval(inches)

4.2.2. Erosion and sedimentation

Pervious areas

Accumulation/Attachment

$$DET = DETS(t-1) \times (1.0 - AFFIX) + NVSI \quad (\text{eq. A4.10})$$

Where:

DETS = Storage of detached sediment (tons/acre)
 AFFIX = Fraction by which DETS decreases each day as a result of soil compaction
 NVS = Sediment deposition from the atmosphere (lb/acre/day) with a negative value representing removal

Detachment:

$$DET = DELT60 \times (1.0 - CR) \times SMPF \times KRER \times \left(\frac{RAIN}{DELT60} \right)^{JRER} \quad (\text{eq. A4.11})$$

Where:

DET = Sediment detachment from soil matrix by rainfall (tons/ac\interval)
 DELT60 = Number of hours in interval
 SMPF = Supporting management practice factor
 KRER = Detachment coefficient, dependent on soil properties
 RAIN = Rainfall (in/interval)
 JRER = Detachment exponent, dependent on soil properties
 CR = Fraction of the land covered by snow and other cover
 DETS(t) = DETS(t-1) + DET

Scour:

$$SCRSD = \left(\frac{SURO}{(SURS + SURO)} \right) \times DELT60 \times KGER \times \left(\frac{(SURS + SURO)}{DELT60} \right)^{JGER} \quad (\text{eq. A4.12})$$

Where:

KGE = Coefficient for scour of the matrix soil
 KGER = Exponent for scour of the matrix soil

Transport capacity

$$STCAP = DELT60 \times KSER \times \left(\frac{(SURS + SURO)}{DELT60} \right)^{JSER} \quad (\text{eq. A4.13})$$

Where:

STCAP = Capacity for removing detached sediment (tons/acre/interval)
 KSER = Coefficient for transport of detached sediment
 SURS = Surface water storage (inches)
 SURO = Surface outflow of water (inch/interval)
 JSER = Exponent for transport of detached sediment

IF STCAP > DETS, (Sediment limiting)

$$WSSD = DETS \times \frac{SURO}{(SURS + SURO)}$$

IF STCAP < DETS (Transport limiting)

$$WSSD = STCAP \times \frac{SURO}{(SURS + SURO)}$$

Where:

WSSD = Washoff of detached sediment (tons/acre/interval)

$$DES(t) = DETS(t-1) \times (1.0 - AFFIX) + NVSI$$

Where:

DETS = Storage of detached sediment (tons/acre)
 AFFIX = Fraction by which DETS decreases each day as a result of soil compaction
 NVSI = Sediment deposition from the atmosphere (lb/acre/day) with a negative value

representing removal

Impervious areas

No detachment or scouring occurs in impervious areas, only available sediments are transported

Accumulation/Removal

$$SLDS = ACCSDP + SLDSS \times (1.0 - REMSDP) \quad (\text{eq. A4.14})$$

Where:

SLDS	=	Solids in storage at end of day (tons/acre)
ACCSDP	=	Accumulation rate of the solids storage (tons/acre/day)
SLDSS	=	Solids in storage at start of day
REMSDP	=	Unit removal rate of solids storage (fraction removed per day)

Transport capacity

$$STCAP = DELT60 \times KEIM \times \left(\frac{(SURS + SURO)}{DELT60} \right)^{JEIM} \quad (\text{eq. A4.15})$$

Where:

STCAP	=	Capacity for removing solids (tons/ac per interval)
DELT60	=	Hours per interval
KEIM	=	Coefficient for transport of solids
SURS	=	Surface water storage (inches)
SURO	=	Surface outflow of water (in/interval)
JEIM	=	Exponent for transport of solids

When STCAP is greater than the amount of solids in storage, washoff is calculated by:

$$SOSLD = SLDS \times \frac{SURO}{(SURS + SURO)}$$

If the storage is sufficient to fulfill the transport capacity, then the following relationship is used:

$$SOSLD = STCAP \times \frac{SURO}{(SURS + SURO)}$$

Where:

SOSLD	=	Washoff of solids (tons/ac per interval)
SLDS	=	Solids storage (tons/ac)
SOSLD	=	Subtracted from SLDS

4.2.3. Nutrient transformation and transport

a. Nutrient transformation in soil

The main transformation processes of nutrient in soil are: adsorption/desorption, plant uptake, immobilization, mineralization, denitrification, nitrification that are modelled in HSPF¹ as follows:

¹ Since data is not available for simulation (e.g. time series data of soil temperature) the nutrient transformation in soil is not used in this application

Adsorption and desorption

The adsorption/desorption processes for ammonium, organic phosphorus/nitrogen, phosphate are modeled by first-order kinetics or a freundlich isotherm.

First-Order Kinetics method

$$DES = CMAD \times KDS \times THKDS^{(TMP-35)} \quad (\text{eq. A4.16})$$

$$ADS = CMSU \times KAD \times THKAD^{(TMP-35)} \quad (\text{eq. A4.17})$$

Where:

DES	=	Current desorption flux of chemical (mass/area per interval)
CMAD	=	Storage of adsorbed chemical (mass/area)
KDS	=	First-order desorption rate parameter (per interval)
THKDS	=	Temperature correction parameter for desorption
TMP	=	Soil layer temperature (degrees C)
ADS	=	Current adsorption flux of chemical (mass/area per interval)
CMSU	=	Storage of chemical in solution (mass/area)
KAD	=	First-order adsorption rate parameter (per interval)
THKAD	=	Temperature correction parameter for adsorption

THKDS and THKAD are typically about 1.06

Single Value Freundlich

$$X = KF1 \times C^{\left(\frac{1}{N1}\right)} + XFIX \quad (\text{eq. A4.18})$$

Where:

X	=	Chemical adsorbed on soil (ppm of soil)
KF1	=	Single value Freundlich K coefficient
C	=	Equilibrium chemical concentration in solution (ppm of solution)
N1	=	Single value Freundlich exponent
XFIX	=	Chemical which is permanently fixed (ppm of soil)

Nitrogen/phosphorus transformations

Nitrogen transformation processes (denitrification, nitrification, plant uptake, immobilization, mineralization), phosphorus transformation processes (plant uptake, immobilization, mineralization) are modelled using temperature-corrected, first order kinetics with separate constants defined for each soil layer (Donigian et al., 1995).

The optimum first-order kinetic rate parameter is corrected for soil temperatures below 35 degrees C by the generalized equation:

$$KK = K \times TH^{(TMP-35)} \quad (\text{eq. A4.19})$$

Where:

KK	=	Temperature-corrected first-order reaction rate (/interval)
K	=	Optimum first-order reaction rate at 35 degrees C (/interval)
TH	=	Temperature correction coefficient for reaction (typically about 1.06)
TMP	=	Soil layer temperature (degrees C)

Optional Methods for Modeling Plant Uptake of Nitrogen

The monthly target for each soil layer is calculated as:

$$MONTGG = NUPTGT \times NUPTFM(MON) \times NUPTM(MON) \times CRPERC(MON, ICROP)$$

Where:

MONTGT	=	Monthly plant uptake target for current crop (lb N/ac or kg N/ha)
NUPTGT	=	Total annual uptake target (lb N/ac or kg N/ha)
NUPTFM	=	Monthly fraction of total annual uptake target (-)
NUPTM	=	Soil layer fraction of monthly uptake target (-)
CRPFRC	=	Fraction of monthly uptake target for current crop (-)
MON	=	Current month
ICROP	=	Index for current crop

b. Nutrient transport to river

Dissolved nutrient transport

The concentration of dissolved constituents is assumed the same as it is from the original storage (surface, upper ground water, ground water) and will contribute to stream as runoff, interflow and ground water flow.

From runoff

$$SQCM = SSCM \times FSO \quad (\text{eq. A4.20})$$

Where:

SSCM	=	Dissolved chemical in surface storage
FSO	=	Fraction flux in surface layer storage

The fraction of chemical in solution that is transported overland from the surface layer storage (FSO) is the surface moisture outflow divided by the surface layer moisture storage.

From interflow

$$IOCM = ISCM \times FIO \quad (\text{eq. A4.21})$$

Where:

ISCM	=	Dissolved chemical in upper layer transitory (interflow) storage
FIO	=	Fraction flux in upper layer transitory (interflow) storage

From groundwater

$$AOCM = ASCM \times FAO \quad (\text{eq. A4.22})$$

Where:

ASCM	=	Dissolved chemical in active groundwater storage
FAO	=	Fraction flux in active groundwater storage

In HSPF, the percolating of dissolved nutrient is described by the following equation:

$$FSP = SLMPF \times \frac{SDOWN}{SMST} \quad (\text{eq. A4.23})$$

Where:

FSP	=	Fraction of dissolved constituents in the surface zone that percolates (between 0 and 1)
SLMPF	=	Arbitrary reduction factor (<1)
SDOWN	=	Amount of water percolating down (inch)

SMST = Amount of water stored in surface layer (inch)

Percolation of dissolved constituents from the upper zone to the lower zone is calculated as:

$$FUP = \frac{UZS}{UZSN \times ULPF} \times \frac{UDOWN}{UMST} \quad (\text{eq. A4.24})$$

Where:

ULFP = Factor for retarding percolation

UDOWN = Amount of water percolating down (in.)

UMST = Moisture storage (in.)

FUP = Fraction of dissolved constituents from upper zone that percolates (between 0 and 1)

This equation can be also applied for the percolation from lower zone to ground water storages (Bicknell et al., 2001; Radcliffe and Lin, 2007)

Particulate nutrient transport

In HSPF, the particular constituent removed from the land surface is assumed to be proportional to the solids removal. Thus, the removal of particulate nutrients (adsorbed ammonium and phosphate) and organic form of the nutrients by solids washoff are simulated by:

- Removal associated constituents by detached sediment transport

$$WASHQS = WSSD \times POTFW \quad (\text{eq. A4.25})$$

Where:

WASHQS = Flow of quality constituents associated with detached sediment washoff (quantity/arc per interval)

WSSD = Washoff detached sediment (calculated from erosion section)

POTFW = Washoff potency factor (quantity/ton) (input calibrated parameter)

- Direct wash-off from the land

$$SQOQ = SQO \times (1 - \exp^{(-SURO + WSFAC)}), \text{ quantity/ac per interval} \quad (\text{eq. A4.26})$$

Where:

SURO = Surface runoff in water (in) per interval

SQO = Storage of available quality constituent on the surface (mass/area) (input calibrated parameter), accumulated and updated SQO is calculated in eq. A4.24

WSFAC = Susceptibility of the quality constituent to washoff (/inch)

$$WSFAC = \frac{2.30}{WSQOP}$$

WSQOP = Rate of surface runoff that results in 90 percent washoff in one hour (in/hr) (input calibrated parameter)

If atmospheric deposition data are input to the model, the storage is updated as follows:

$$SQO = SQO + ADFX + PREC \times ADCN \quad (\text{eq. A4.27})$$

Where:

SQO = Storage of available quality constituent on the surface (mass/area) (input calibrated parameter)

ADFX = Dry or total atmospheric deposition flux (mass/area per interval)

PREC = Precipitation depth

ADCN = Concentration for wet atmospheric deposition (mass/volume)

If the storage is updated once a day to account for accumulation and removal which occurs independent of runoff by the equation:

$$SQO = ACQOP + SQOS \times (1 - REMQOP) \quad (\text{eq. A4.28})$$

Where:

ACQOP = Accumulation rate (quantity/ arc per Day) (input calibrated parameter)
 REMQOP = Unit removal rate of the stored constituent (per Day)

$$REMQOP = \frac{ACQOP}{SQOLIM}$$

SQOLIM = Asymptotic limit for SQO as time approaches infinity (quantity/ac), if no washoff occurs (or SQO - the maximum storage of QUALOF if QSOFG is positive) (input calibrated parameter)

If the accumulation and removal occur every interval, the removal rate removal rate is applied to atmospheric deposition and lateral inflows, as well as the accumulation rate and is recomputed every interval as:

$$REMOV = REMQOP + \frac{INTOT}{\left(\frac{ACQOP}{REMQOP} \right)} \quad (\text{eq. A4.29})$$

Where:

INTOT = Total of atmospheric deposition and lateral inflow
 REMOV = Removal rate
 DELT60 = Number of hours per interval

Then storage is updated as:

$$SQO = ACQOP \times \left(\frac{DELT60}{24.0} \right) + SQO \times (1.0 - REMOV)^{\left(\frac{DELT60}{24.0} \right)} \quad (\text{eq. A4.30})$$

4.2.4. River routing

b. Sediment routing

SEDTRN section in RCHRES module simulate inorganic sediment load into three components which are sand, silt, and clay. Sand transport is simulated by Toffaleti method, Colby method, and Power function method.

Sand transport simulation – Power function

$$PSAND = KSAND \times (AVVELE)^{EXPSND} \quad (\text{eq. 4.31})$$

Where:

PSAND = Potential sand concentration
 AVVELE = Average velocity
 KSAND = Coefficient (input parameter)
 EXPSND = Exponent (input parameter)

Scour/Deposition for cohesive sediments (silt and clay)

$$\text{Scour Rate: } S = M \times \left(\frac{TAU}{TAUCS} - 1.0 \right) \quad (\text{eq. 4.32})$$

$$\text{Deposit Rate: } D = W \times CONC \times \left(1.0 - \frac{TAU}{TAUCD} \right) \quad (\text{eq. 4.33})$$

Shear Stress: $TAU = SLOPE \times GAM \times HRAD$

Where:

M	=	Erodibility coefficient (lb/ft ² /hr)
TAUSC	=	Critical shear stress for scour (lb/ft ²)
TAUCD	=	Critical shear stress for deposition (lb/ft ²)
CONC	=	Suspended sediment (lb/ft ³)
GAM	=	Density of water (lb/ft ³)
HRAD	=	Hydraulic radius

c. Nutrient routing

The typical algorithms related nutrient transformation processes are as follows:

Benthic Release

$$RELEAS = BRCON(I) \times SCRFAS \times DEPCOR \quad (\text{eq. 4.34})$$

Where:

RELEAS	=	Amount of constituent released (mg/ L per interval)
BRCON(I)	=	Benthic release rate (BRTAM or BRPO4) for constituent (mg/m ² per interval)
SCRFAC	=	Scouring factor, dependent on average velocity of the water
DEPCOR	=	Conversion factor from mg/m ² to mg/ L

Nitrification

$$TAMNIT = KTAM20 \times (TCNIT)^{TW-20} \times TAM \quad (\text{eq. 4.35})$$

Where:

TAMNIT	=	Amount of NH ₃ oxidation (mg N/L per interval)
KTAM20	=	Ammonia oxidation rate coefficient at 20 oC (/interval)
TCNIT	=	Temperature correction coefficient, defaulted to 1.07
TW	=	Water temperature (oC)
TAM	=	Total ammonia concentration (mg N/L)

Adsorption/Desorption of Ammonia and Orthophosphorus

$$SNUT(J) = DNUT \times ADPM(J) \quad (\text{eq. 4.35})$$

Where:

SNUT(J)	=	Equilibrium concentration of adsorbed nutrient on sediment fraction J (mg/kg)
DNUT	=	The equilibrium concentration of dissolved nutrient (mg/L)
ADPM(J)	=	Adsorption parameter (or Kd) for sediment fraction J (l/kg) J=1; 2; 3 for sand; silt; clay, respectively

4.3. Model parameters

4.3.1. Hydrology

Table A4.1: Process and physical parameters used after calibration of the HSPF model for hydrology

Process parameter	Description (units)	Parametric values					
		Forest	Urban and road	Cropland & pasture	Rice	Trees	Wetland
LZSN	Lower zone nominal storage (mm)	381	482	482	482	482	482
INTFW	Interflow inflow parameter	1.5	1.5	1.5	1.5	1.5	1.5
INFILT	Index to soil infiltration capacity (mm/h)	2.44	1.22	12.69	1.71	6.34	0.24
AGWRC	Groundwater recession coefficient (1/day)	0.99	0.99	0.99	0.99	0.99	0.99
UZSN	Upper zone nominal storage (mm)	4.5	7.7	7.7	7.7	7.7	7.7
IRC	Interflow recession parameter	0.3	0.3	0.5	0.5	0.5	0.5

Process parameter	Description (units)	Parametric values					
		Forest	Urban and road	Cropland & pasture	Rice	Trees	Wetland
LZETP	Lower zone ET parameter	0.6	0.3	0.6	0.8	0.7	0.9
LSUR	Length of overland flow plane (m)	45	50	45	37	55	15
SLSUR	Slope of overland flow plane	0.41	0.02	0.02	0.02	0.02	0.02
NSUR	Manning's n for the overland flow	0.15	0.1	0.25	0.4	0.3	0.08

4.3.2. Sediment

Table A4.2: Sediment yield parameters used after calibration of the HSPF model

Process parameter	Description (units)	Parametric values					
		Forest	Urban and road	Cropland and pasture	Rice	Trees	Wetland
KRER	Coefficient in the soil detachment equation	0.3	0.3	0.25	0.2	0.25	0.2
JRER	Exponent in the soil detachment equation (<i>default values</i>)	2	2	2	2	2	2
COVER	The fraction of land surface which is shielded from erosion by rainfall	0.8	0.9	0.7	0.5	0.6	0.2
AFFIX	Fraction by which detached sediment storage decreases each day as a result of soil compaction	0.05	0.05	0.05	0.05	0.05	0.05
NVSI	Rate at which sediment enters detached storage from the atmosphere	0	0	0	0	0	0
KSER	Coefficient in the detached sediment washoff equation (Diaz-Ramirez et al., 2008)	10	10	10	10	10	10
JSER	Exponent in the detached sediment washoff equation (<i>default values</i>)	2	2	2	2	2	2

4.3.3. Nutrients

Table A4.3: Nutrient parameters (P-PO4) used after calibration of the HSPF model

Process parameter	Description	Parametric values					
		Forest	Urban and road	Cropland and pasture	Rice	Trees	Wetland
SQO	Initial storage of QUALOF on the surface of the PLS (kg/ha)	0.45	0.45	0.45	0.45	0.45	0.45
POTFW	Washoff potency factor for a QUALSD (kg/ton)	0.03	0.37	0.07	0.2	0.13	0.2
POTFS	Scour potency factor for a QUALSD (kg/ton)	0.02	0.17	0.03	0.09	0.06	0.09
ACQOP	Rate of accumulation of QUALOF (kg/ha.day)	0.045	0.002	0.054	0.045	0.045	0.045
SQOLIM	SQOLIM is the maximum storage of QUALOF, (kg/ha) (<i>recommended value</i>)	0.027	0.027	0.027	0.027	0.027	0.027
WSQOP	Rate of surface runoff which will remove 90 percent of stored QUALOF per hour (<i>recommended value</i>)	0.5	0.5	0.5	0.5	0.5	0.5
MON-ACCUM	Monthly values of accumulation rate of QUALOF at start of each month (kg/ha.day)	0.05	0.05	0.05	0.05	0.05	0.05
MON-SQOLIM	Monthly values limiting	0.45	0.45	0.45	0.45	0.45	0.45

Process parameter	Description	Parametric values					
		Forest	Urban and road	Cropland and pasture	Rice	Trees	Wetland
	storage of QUALOF at start of each month (from July to September) (kg/ha)						

Table A4.4: Nutrient parameters (N-NH4) used after calibration of the HSPF model

Process parameter	Description (units)	Parametric values					
		Forest	Urban and road	Cropland and pasture	Rice	Trees	Wetland
SQO	Initial storage of QUALOF on the surface of the PLS (kg/ha)	0.71	0.71	0.71	0.71	0.71	0.71
POTFW	Washoff potency factor for a QUALSD (kg/ton)	0.03	0.24	0.09	0.18	0.12	0.24
POTFS	Scour potency factor for a QUALSD (kg/ton)	0.02	0.12	0.05	0.09	0.06	0.09
ACQOP	Rate of accumulation of QUALOF (kg/ha.day)	0.22	0.01	0.27	0.22	0.22	0.01
SQOLIM	SQOLIM is the maximum storage of QUALOF (kg/ha) (<i>recommended value</i>)	0.062	0.062	0.062	0.062	0.062	0.062
WSQOP	Rate of surface runoff which will remove 90 percent of stored QUALOF per hour (<i>recommended value</i>)	0.5	0.5	0.5	0.5	0.5	0.5
MON-ACCUM	Monthly values of accumulation rate of QUALOF at start of each month (kg/ha.day)	0.05	0.05	0.05	0.05	0.05	0.05
MON-SQOLIM	Monthly values limiting storage of QUALOF at start of each month (from July to September) (kg/ha)	0.45	0.45	0.45	0.45	0.45	0.45

Table A4.5: Nutrient parameters (N-NO3) used after calibration of the HSPF model

Process parameter	Description (units)	Parametric values					
		Forest	Urban and road	Cropland and pasture	Rice	Trees	Wetland
SQO	Initial storage of QUALOF on the surface of the PLS (kg/ha)	2.68	2.68	2.68	2.68	2.68	2.68
POTFW	Washoff potency factor for a QUALSD (kg/ton)	0.02	0.11	0.3	0.09	0.24	0.09
POTFS	Scour potency factor for a QUALSD (kg/ton)	0.01	0.05	0.15	0.05	0.12	0.05
ACQOP	Rate of accumulation of (kg/ha.day)	0.13	0.07	0.19	0.13	0.16	0.13
SQOLIM	SQOLIM is the maximum storage of QUALOF if QSOFG is positive, (kg/ha) (<i>recommended value</i>)	0.223	0.223	0.223	0.223	0.223	0.223
WSQOP	Rate of surface runoff which will remove 90 percent of stored QUALOF per hour (<i>recommended value</i>)	0.5	0.5	0.5	0.5	0.5	0.5

Process parameter	Description (units)	Parametric values					
		Forest	Urban and road	Cropland and pasture	Rice	Trees	Wetland
MON-ACCUM	Monthly values of accumulation rate of QUALOF at start of each month (kg/ha.day)	0.05	0.05	0.05	0.05	0.05	0.05
MON-SQOLIM	Monthly values limiting storage of QUALOF at start of each month (from July to September) (kg/ha)	0.45	0.45	0.45	0.45	0.45	0.45

4.4. Model results

4.4.1. Hydrology

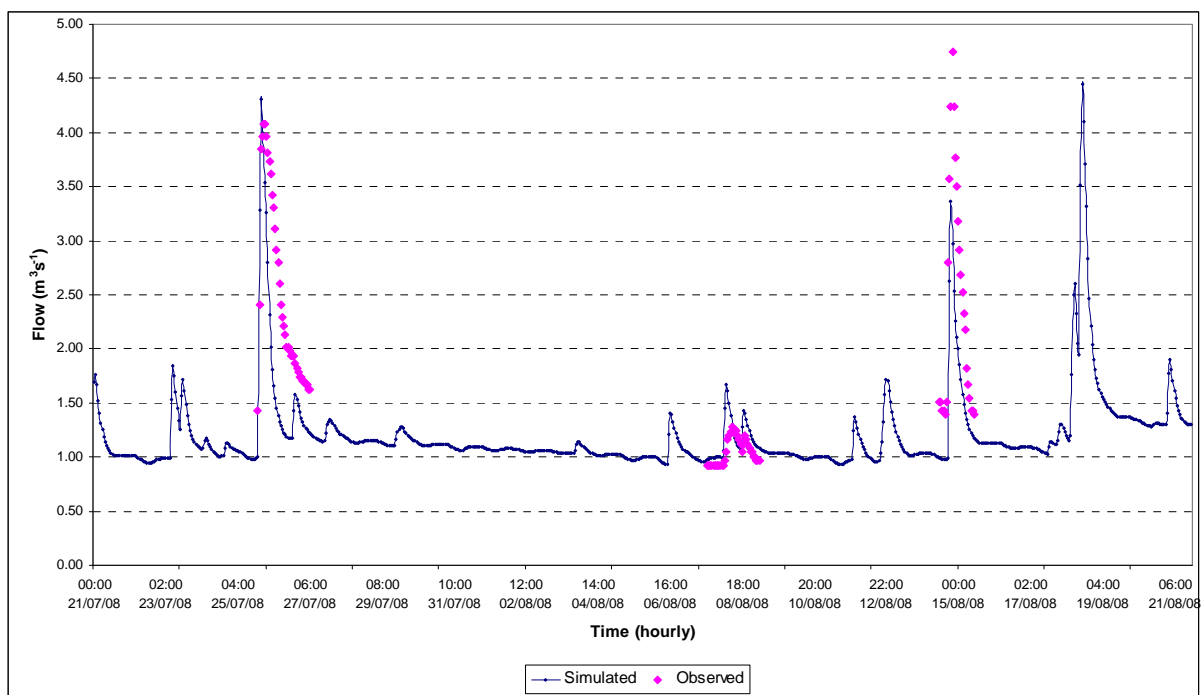


Figure A4.14: Observed and simulated hydrograph from HSPF model (21/7/2008 – 20/8/2008)

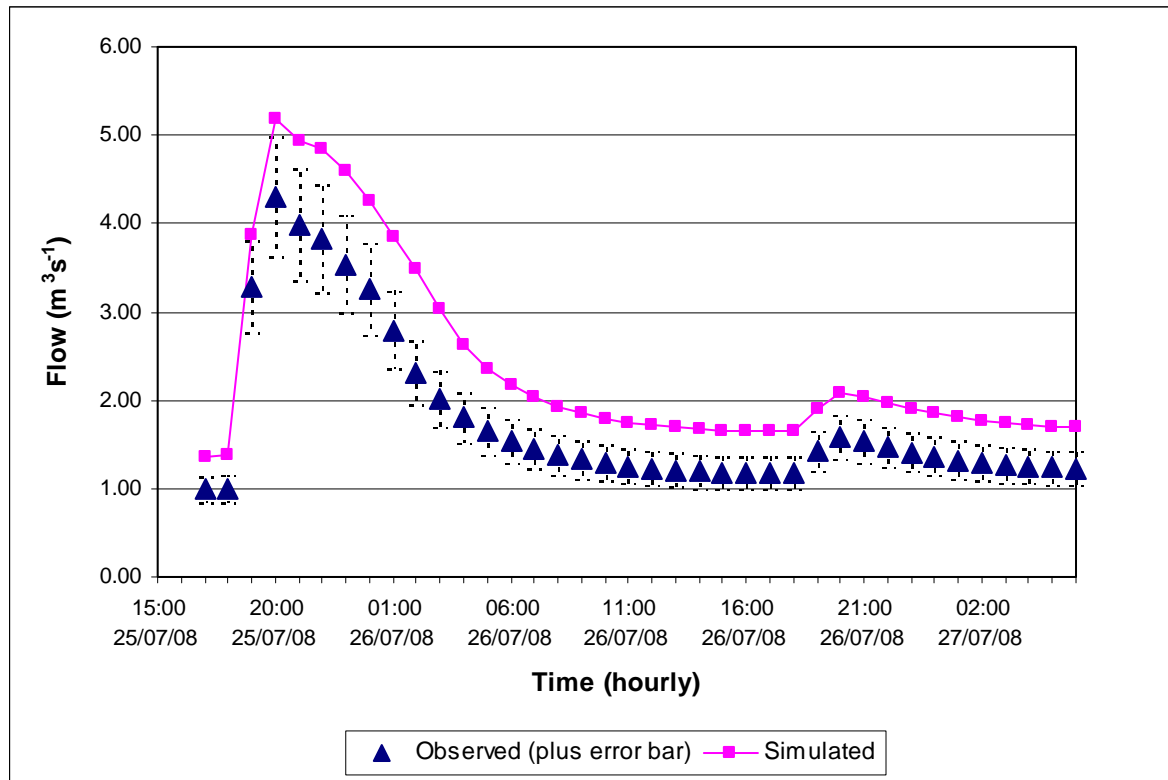


Figure A4.15: Observed and simulated hydrograph from HSPF model (25/7/2008 – 27/7/2008)

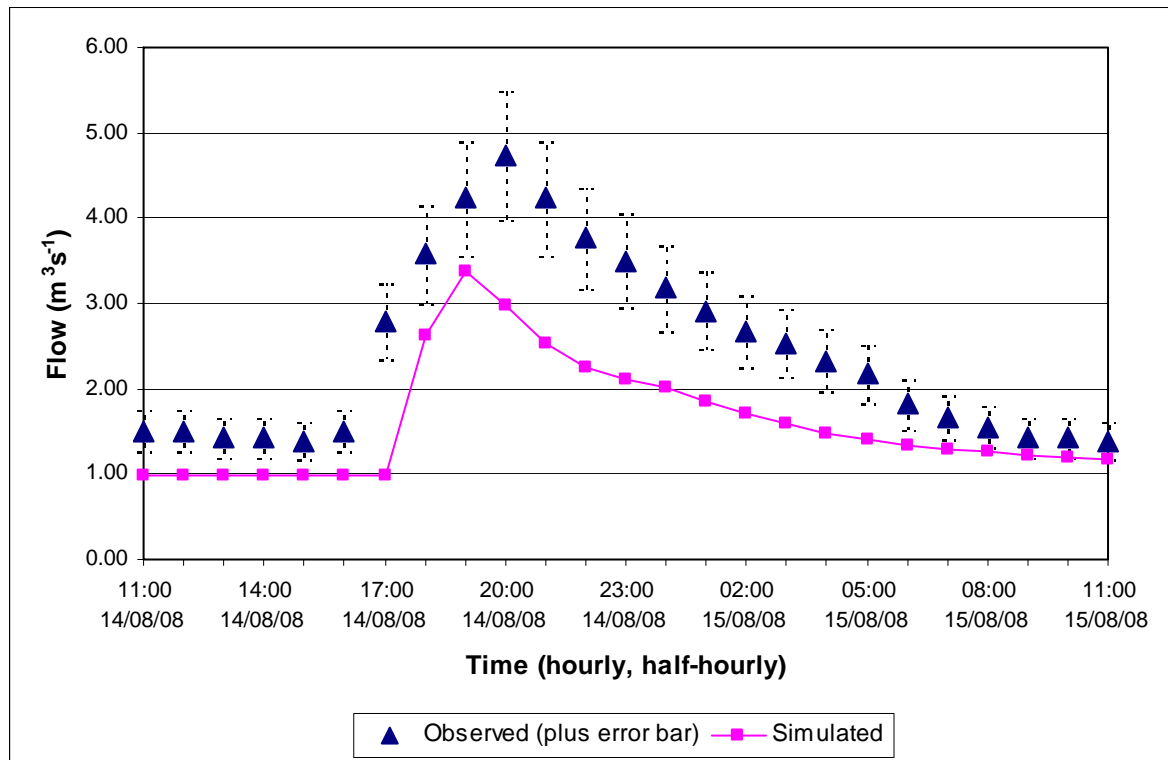


Figure A4.16: Observed and simulated hydrograph from HSPF model (7/8/2008 – 9/8/2008)

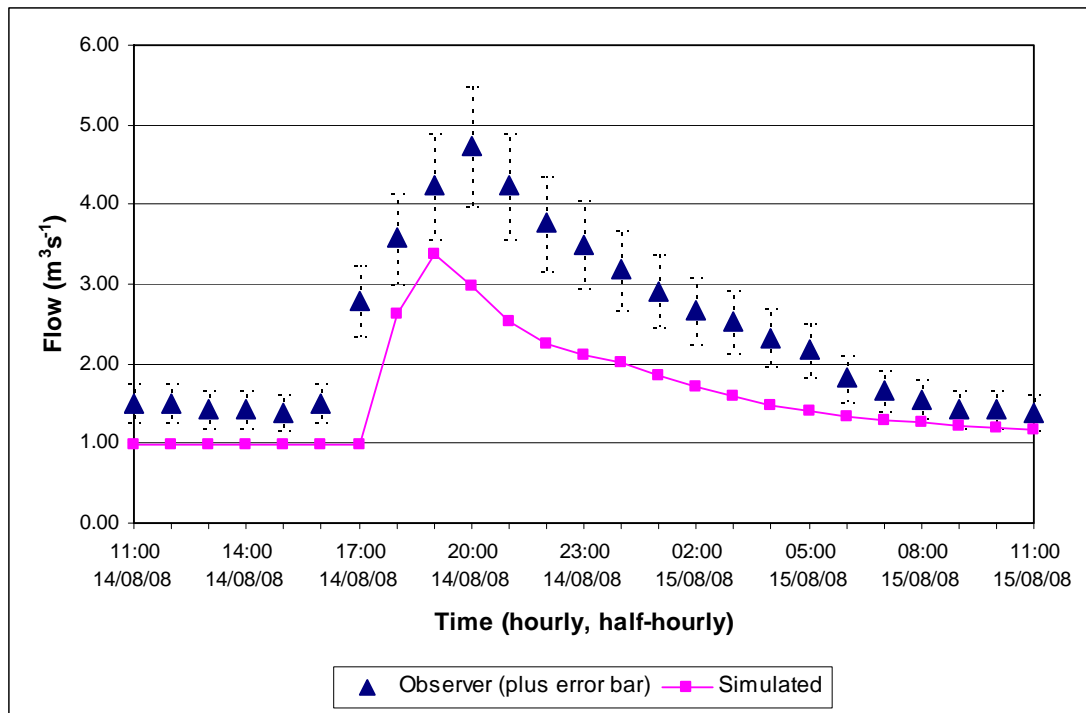


Figure A4.17: Observed and simulated hydrograph from HSPF model (14/8/2008 – 15/8/2008)

4.4.2. Sediments

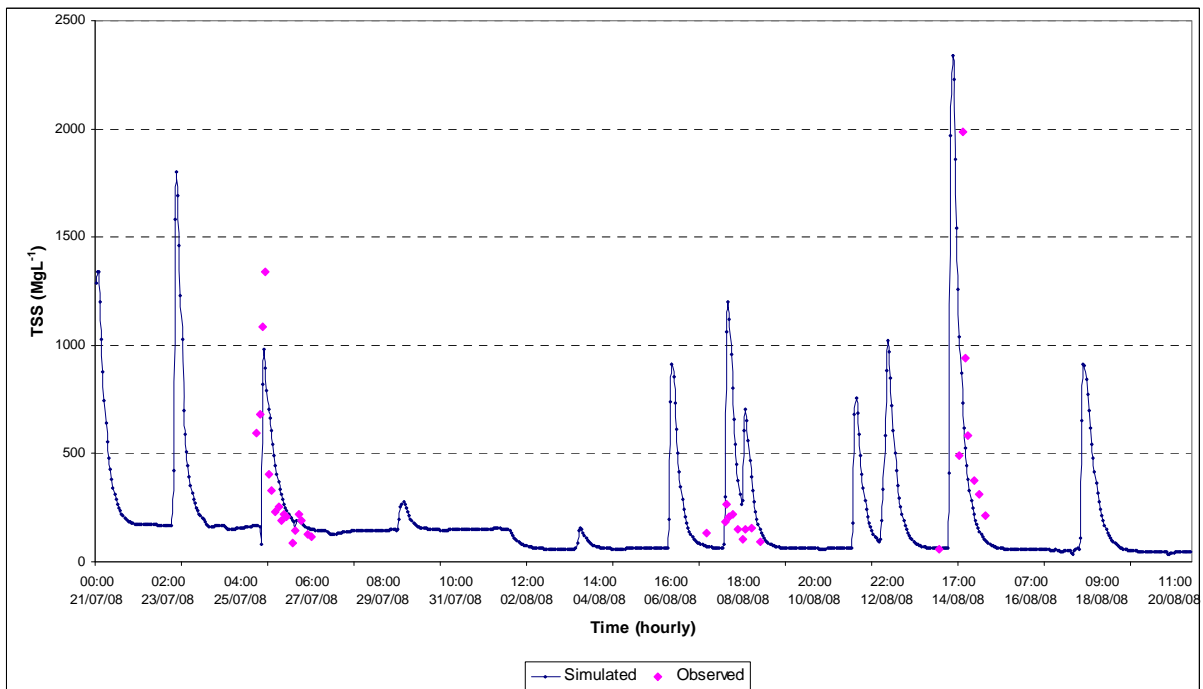


Figure A4.18: Observed and simulated TSS from HSPF model (21/7/2008 – 20/8/2008)

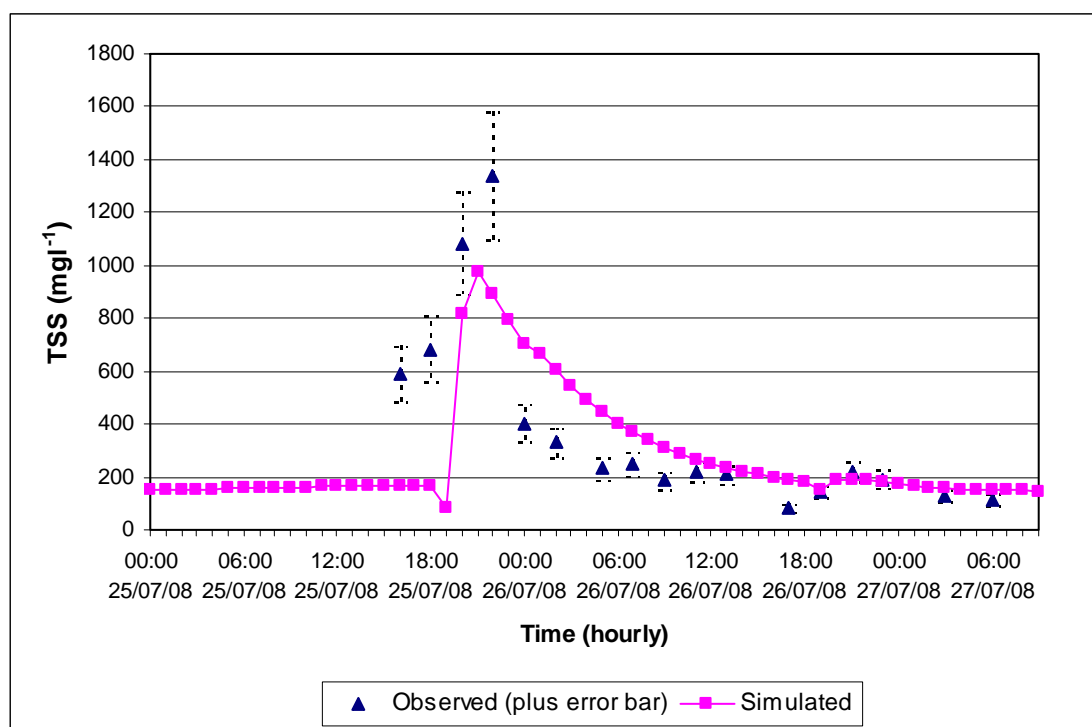


Figure A4.19: Observed and simulated TSS from HSPF model (25/7/2008 – 27/7/2008)

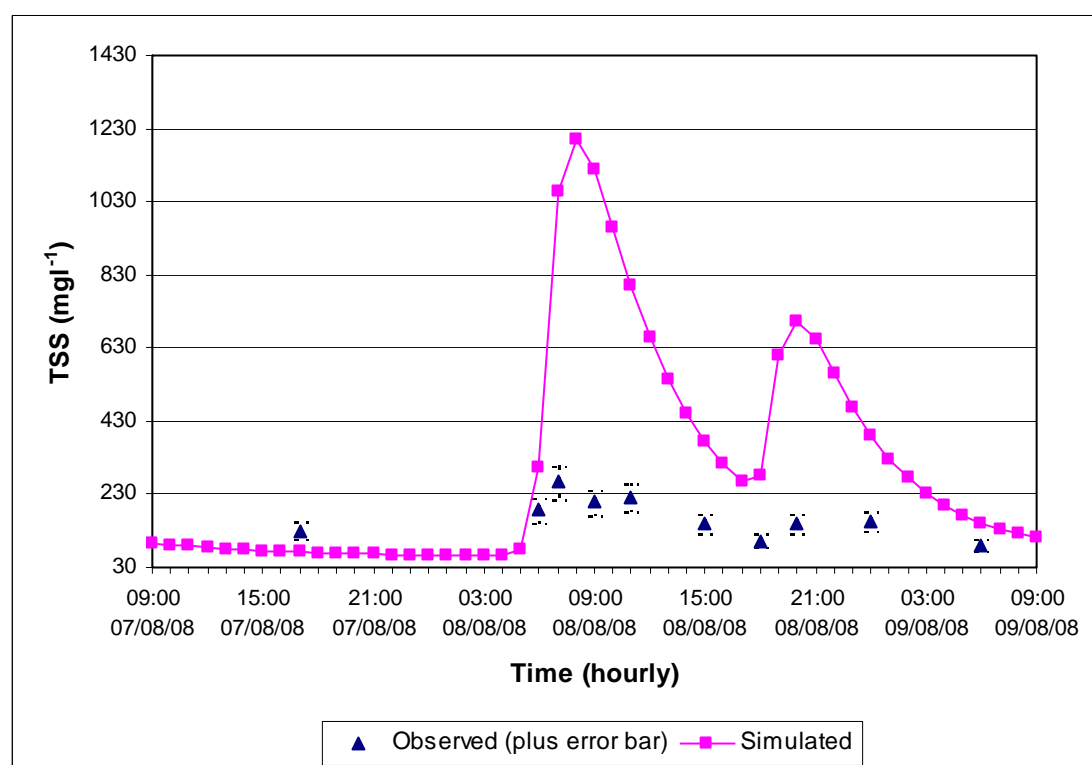


Figure A4.20: Observed and simulated TSS from HSPF model (7/8/2008 – 9/8/2008)

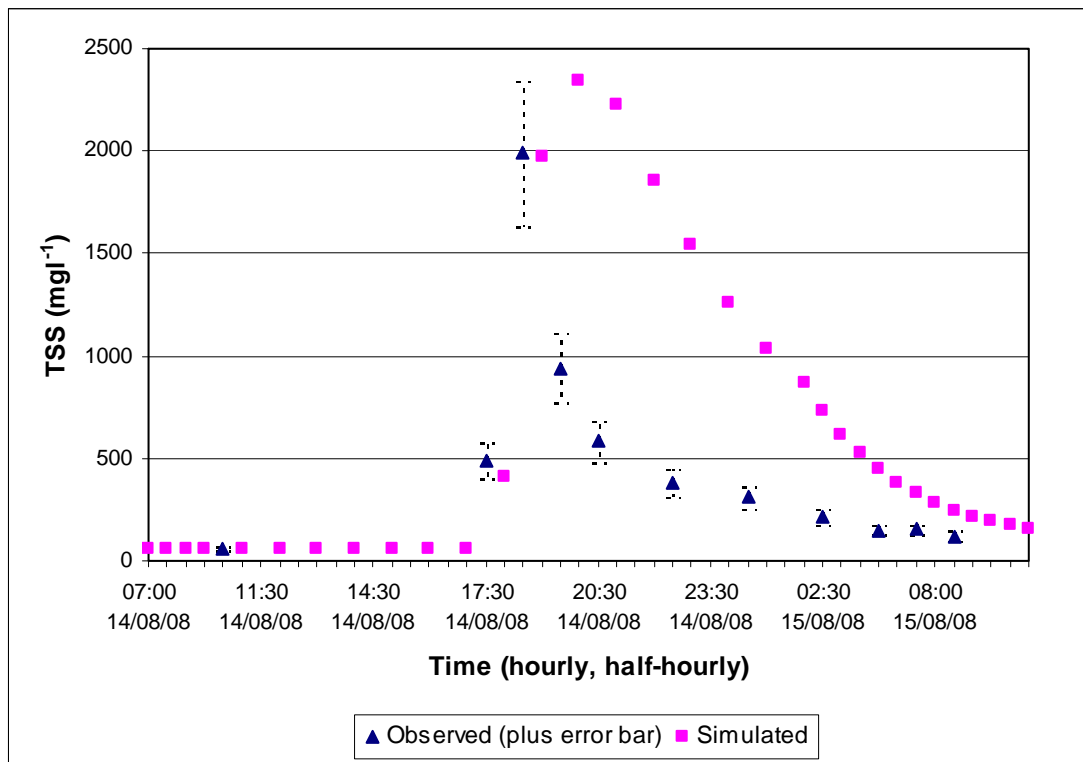


Figure A4.21: Observed and simulated TSS from HSPF model (14/8/2008 – 15/8/2008)

4.4.3. Nutrients

4.4.3.1. Phosphate phosphorus (P-PO_4)

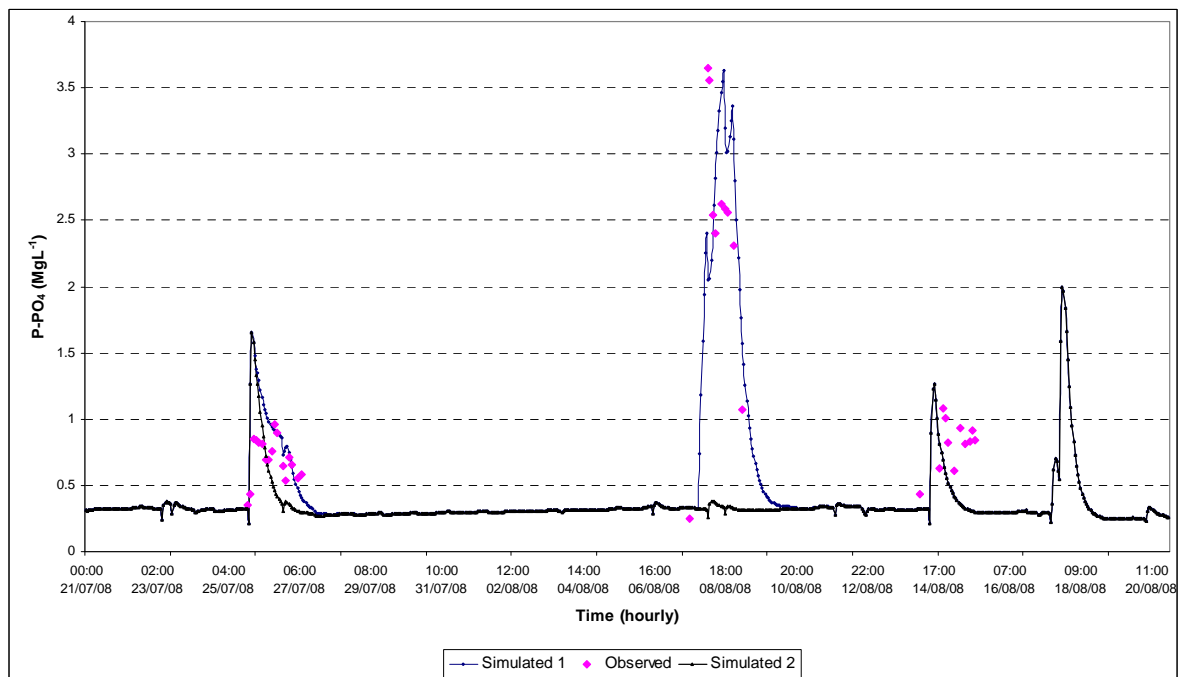


Figure A4.22: Observed and simulated P-PO_4 from HSPF model (21/7/2008 – 20/8/2008)

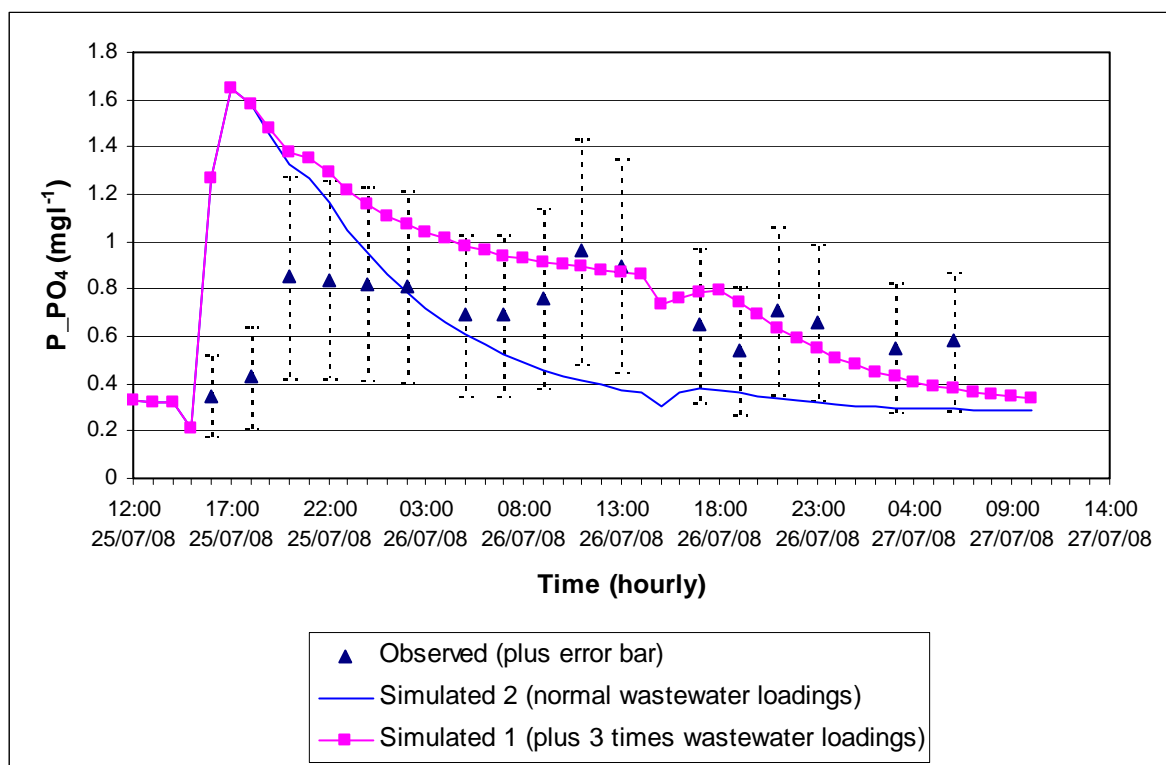


Figure A4.23: Observed and simulated P-PO₄ from HSPF model (25/7/2008 – 27/7/2008)

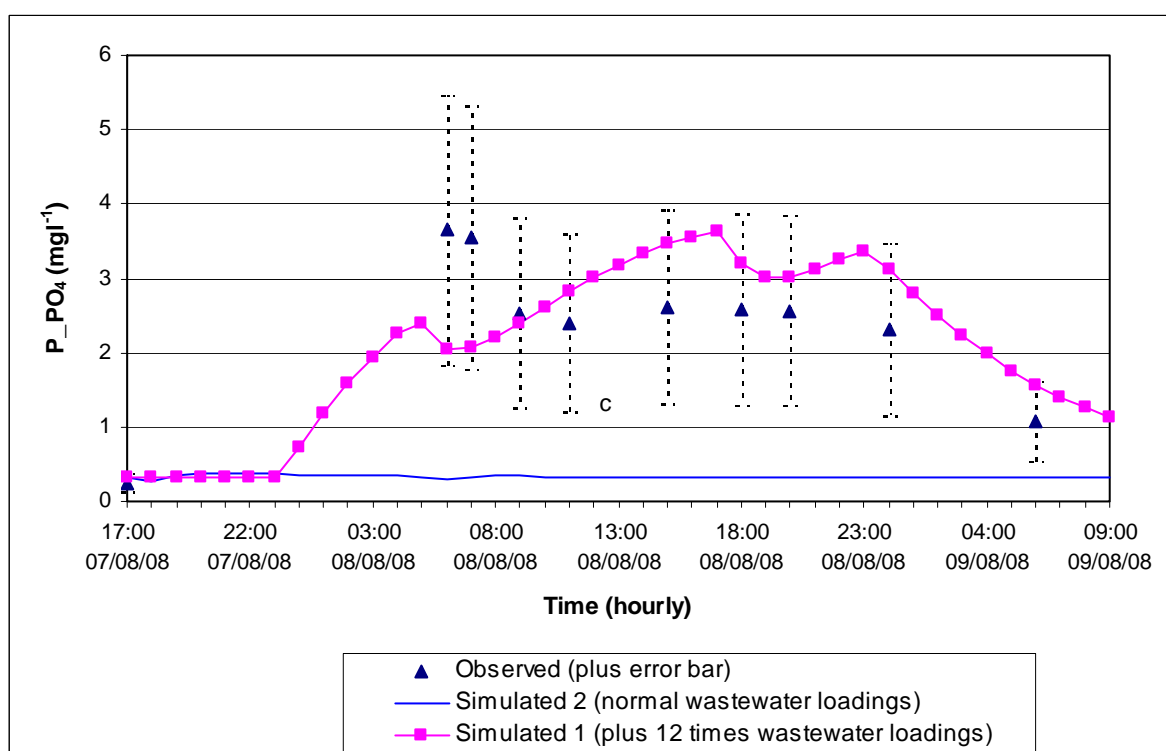


Figure A4.24: Observed and simulated P-PO₄ from HSPF model (7/8/2008 – 9/8/2008)

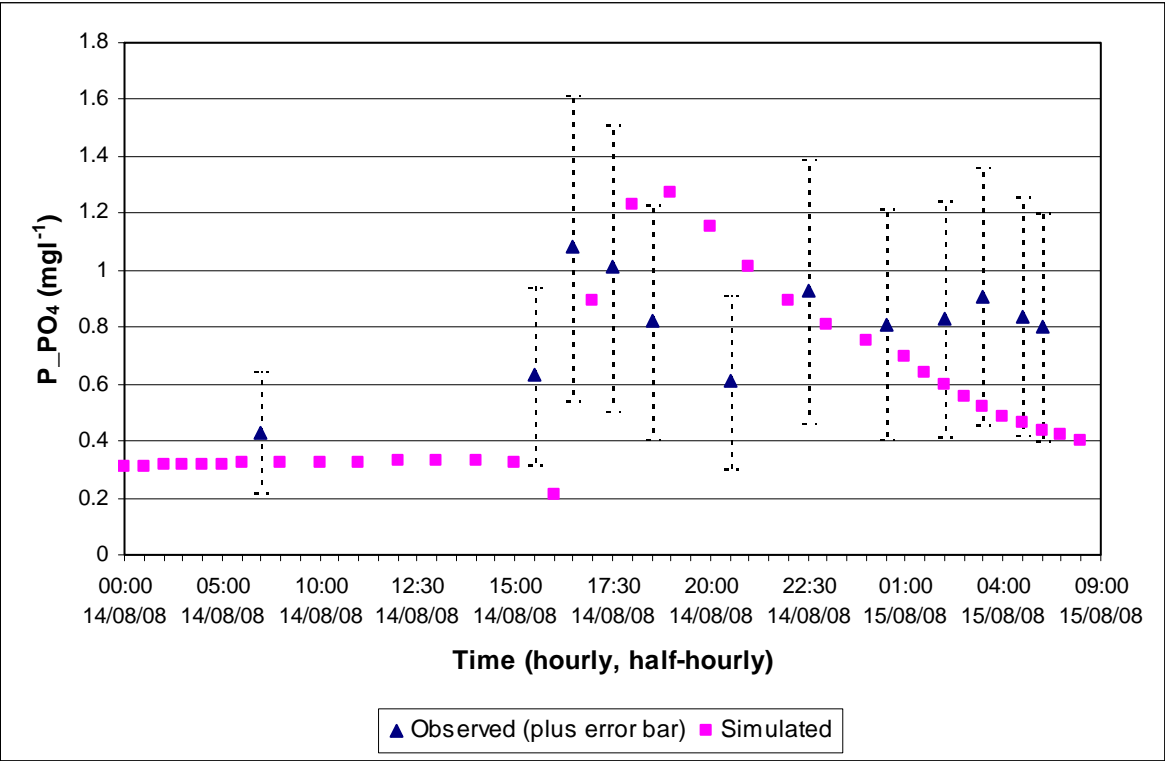


Figure A4.25: Observed and simulated P-PO₄ from HSPF model (14/8/2008 – 15/8/2008)

4.4.3.2. Ammonium nitrogen (N-NH₄)

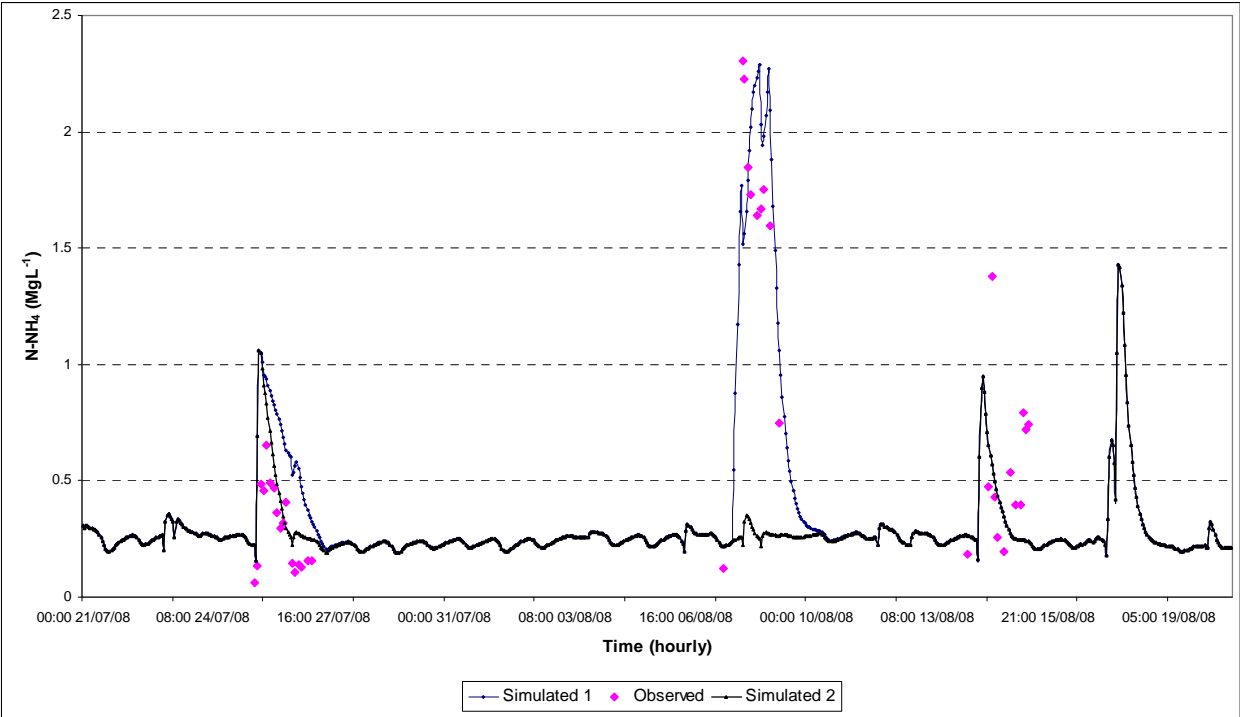


Figure A4.26: Observed and simulated N-NH₄ from HSPF model (21/7/2008 – 20/8/2008)

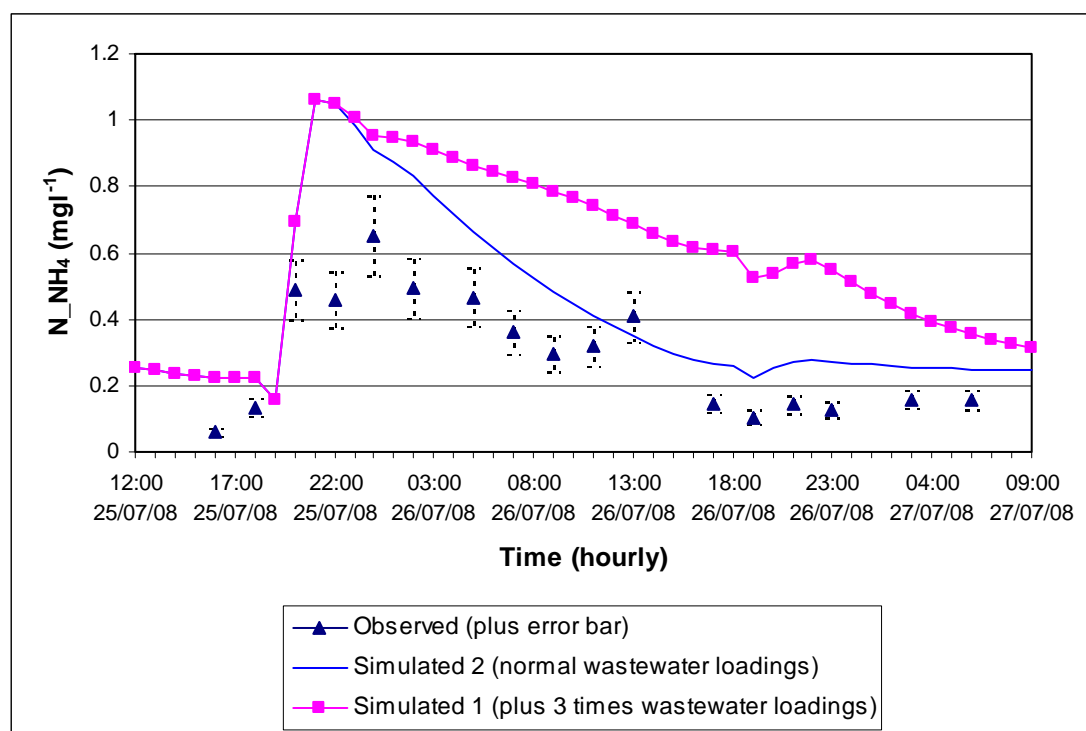


Figure A4.27: Observed and simulated N-NH₄ from HSPF model (25/7/2008 – 27/7/2008)

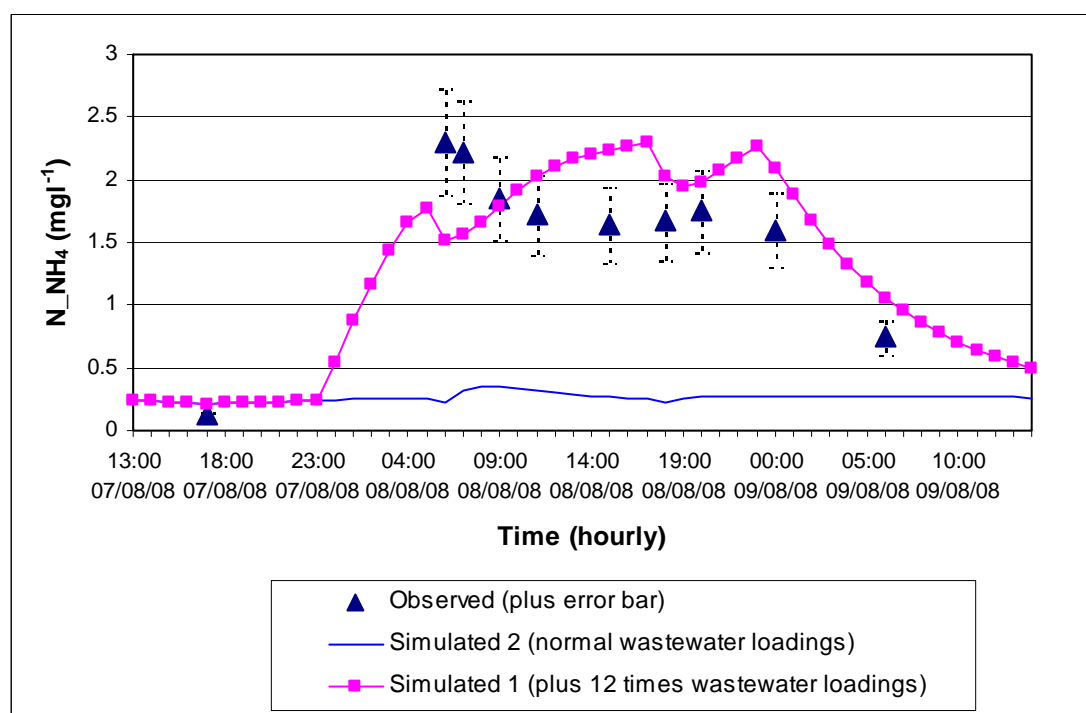


Figure A4.28: Observed and simulated N-NH₄ from HSPF model (7/8/2008 – 9/8/2008)

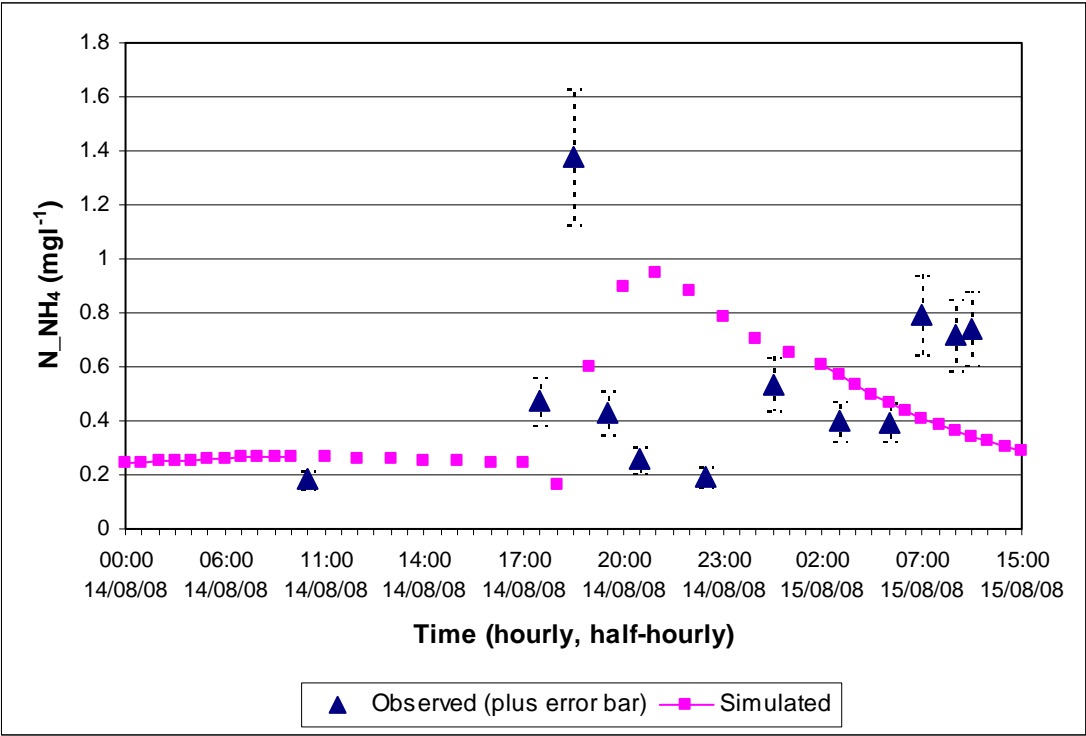


Figure A4.29: Observed and simulated N-NH4 from HSPF model (14/8/2008 – 15/8/2008)

4.4.3.3. Nitrate Nitrogen (N-NO₃)

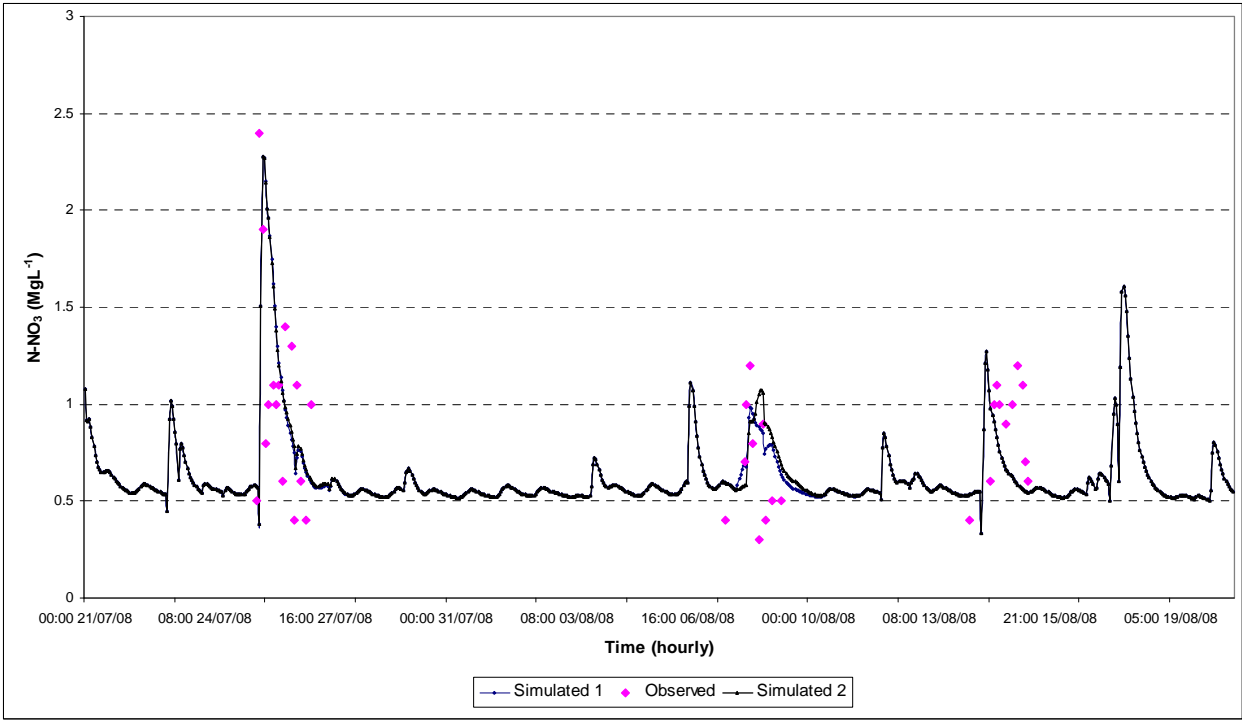


Figure A4.30: Observed and simulated N-NO3 from HSPF model (21/7/2008 – 20/8/2008)

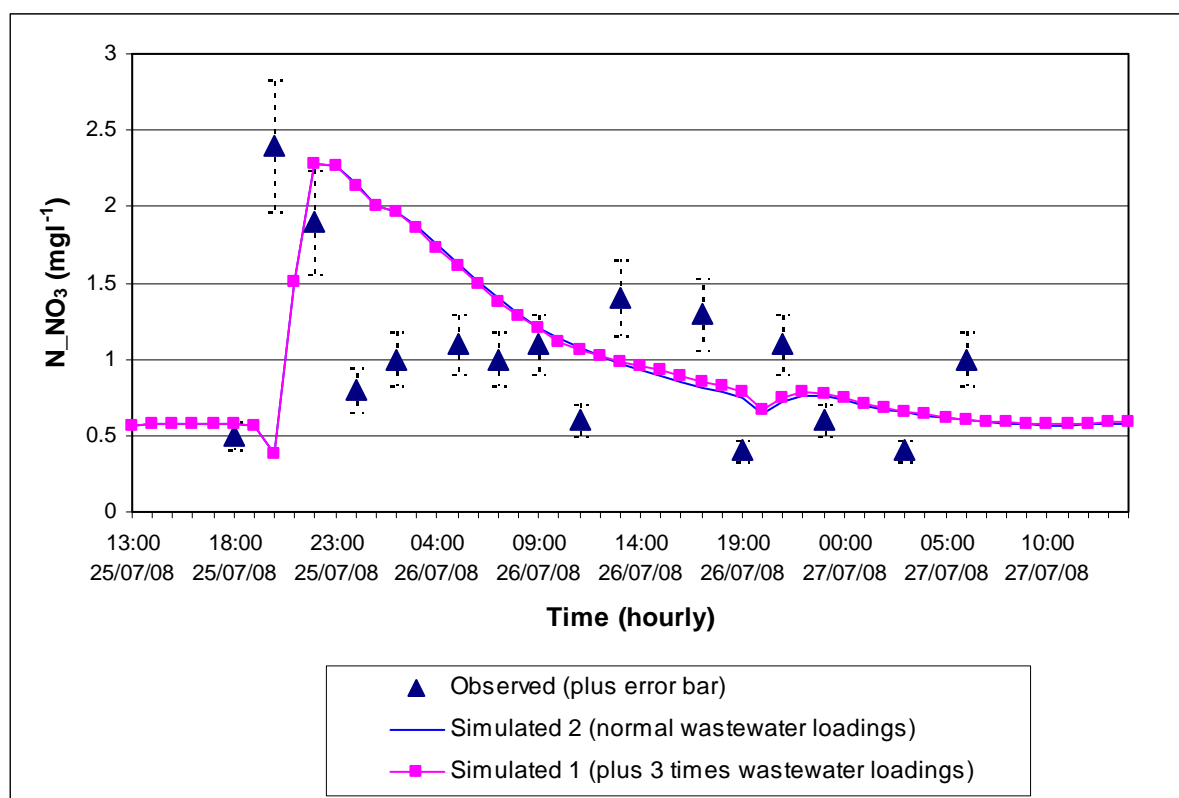


Figure A4.31: Observed and simulated N-NO₃ from HSPF model (25/7/2008 – 27/7/2008)

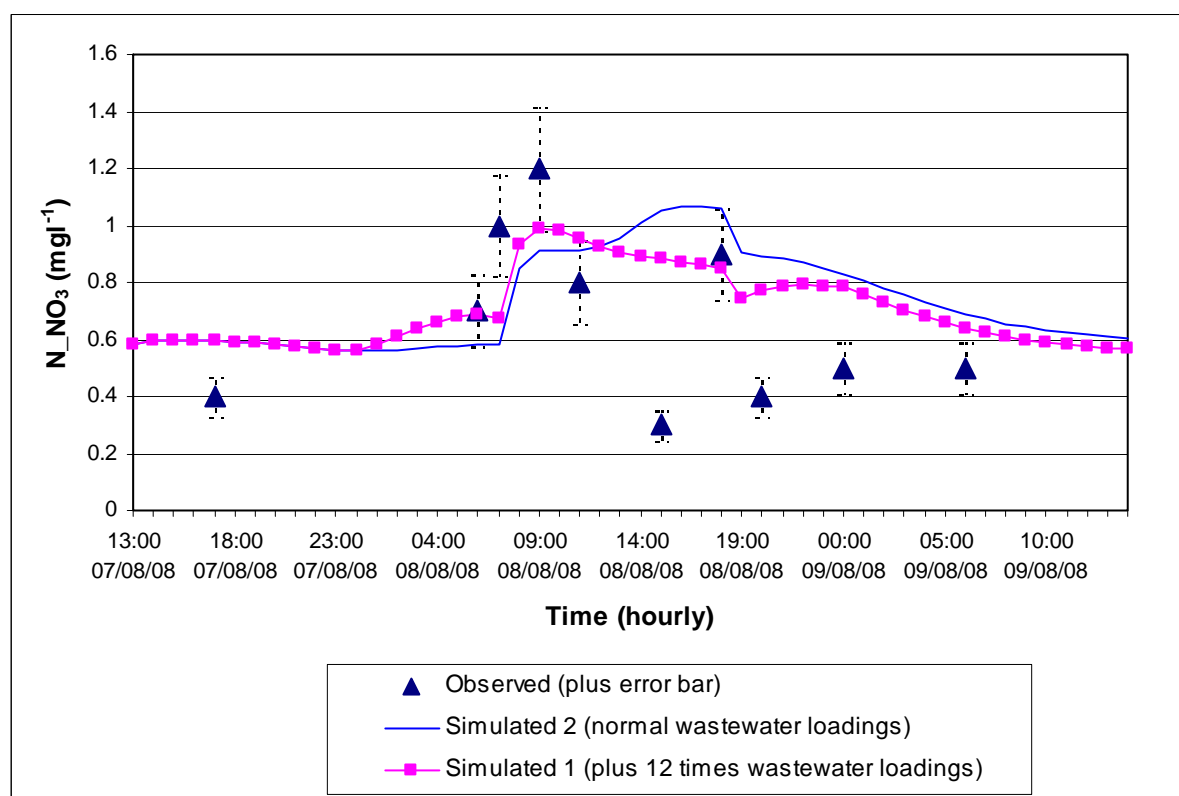


Figure A4.32: Observed and simulated N-NO₃ from HSPF model (7/8/2008 – 9/8/2008)

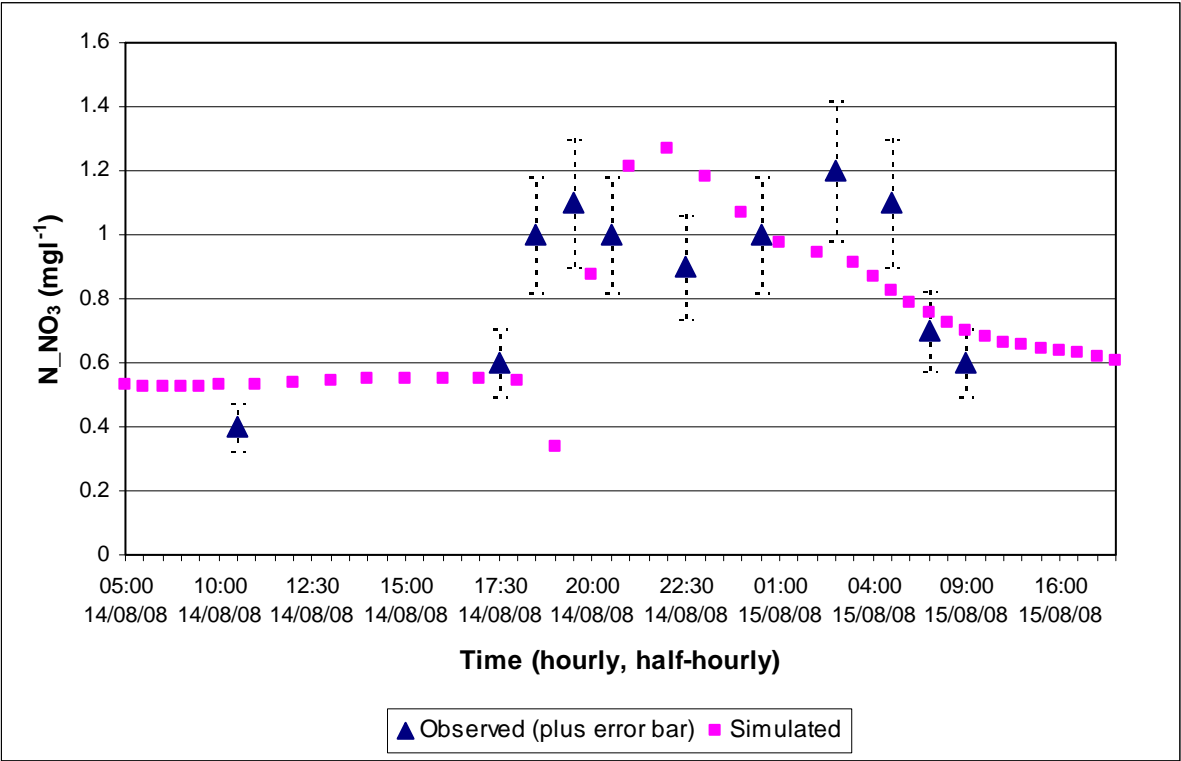


Figure A4.33: Observed and simulated N-NO3 from HSPF model (14/8/2008 – 15/8/2008)

5. Appendix 5: Additional information on the SINUDYM

5.1. Detailed expression of the probability functions applied in the GIUH approach

1. The initial state probability θ_j

$$\theta_1 = \frac{N_1 \bar{A}_1}{A_\Omega} \quad (\text{eq. A5.1})$$

$$\theta_\omega = \frac{N_1}{A_\Omega} \left[\bar{A}_\omega - \sum_{j=1}^{\omega-1} \bar{A}_j \left(\frac{N_j P_{j\omega}}{N_\omega} \right) \right] \quad (\text{eq. A5.2})$$

2. The transition probabilities p_{ij}

The transition probabilities can be approximated as a function of the number of Strahler streams of each order N_i :

$$p_{ij} = \frac{(N_i - 2N_{i+1})E(j, \Omega)}{\sum_{k=i+1}^{\Omega} E(k, \Omega) N_i} + 2 \frac{N_{i+1}}{N_i} \delta_{i+1, j} \quad 1 \leq i \leq j \leq \Omega \quad (\text{eq. A5.3})$$

$\delta_{i+1, j} = 1$ if $j=i+1$ and 0 otherwise. $E(j, \Omega)$ denotes the mean number of interior links of order i in a finite network of order Ω .

$$E(j, \Omega) = N_i \prod_{j=2}^i \frac{(N_{j-1} - 1)}{2N_j - 1}, \quad i=2, \dots, \Omega. \quad (\text{eq. A5.4})$$

An interior link is a segment of channel network between two successive junctions or between the outlet and the first junction up-streams.

For a **3rd order catchment** the initial and transition probability can be expressed as:

$$\theta_1 = \frac{R_B^2}{R_A^2} \quad (\text{eq. A5.5})$$

$$\theta_2 = \frac{R_B}{R_A} - \frac{R_B^3 + 2R_B^2 - 2R_B}{R_A^2(2R_B - 1)} \quad (\text{eq. A5.6})$$

$$\theta_3 = 1 - \frac{R_B}{R_A} - \frac{R_B^3 - 3R_B^2 + 2R_B}{R_A^2(2R_B - 1)} \quad (\text{eq. A5.7})$$

$$p_{12} = \frac{R_B^2 + 2R_B^2 - 2}{2R_B^2 - R_B} \quad (\text{eq. A5.8})$$

$$p_{13} = \frac{R_B^2 - 3R_B + 2}{2R_B^2 - R_B} \quad (\text{eq. A5.9})$$

$$P_{23} = 1$$

For a 4th order catchment the initial and transition probability and the possible paths can be expressed as:

$$\theta_1 = \frac{R_B^3}{R_A^3} \quad (\text{eq. A5.10})$$

$$\theta_2 = \frac{R_B^2}{R_A^2} \left(1 - \frac{R_B}{R_A} \left(\frac{2}{R_B} + \frac{(2R_B - 1)(R_B^2 - 2R_B)}{R_B^2(2R_B - 1) + R_B(R_B^2 - 1) + (R_B^2 - 1)(R_B - 1)} \right) \right) = \frac{R_B^2}{R_A^2} \left(1 - \frac{R_B}{R_A} \times p_{12} \right) \quad (\text{eq. A5.11})$$

$$\theta_3 = \frac{R_B}{R_A} \left(1 - \frac{R_B^2}{R_A^2} \times p_{13} - \frac{R_B}{R_A} \times p_{23} \right) \quad (\text{eq. A5.12})$$

$$\theta_4 = 1 - \left(\frac{R_B}{R_A} \right)^3 \times p_{14} - \left(\frac{R_B}{R_A} \right)^2 \times p_{24} - \left(\frac{R_B}{R_A} \right) \times p_{34} \quad (\text{eq. A5.13})$$

$$p_{12} = \frac{2}{R_B} + \frac{(2R_B - 1)(R_B^2 - 2R_B)}{R_B^2(2R_B - 1) + R_B(R_B^2 - 1) + (R_B^2 - 1)(R_B - 1)} \quad (\text{eq. A5.14})$$

$$p_{13} = \frac{(R_B^2 - 1)(R_B - 1)}{R_B^2(2R_B - 1) + R_B(R_B^2 - 1) + (R_B^2 - 1)(R_B - 1)} \quad (\text{eq. A5.15})$$

$$p_{14} = \frac{(R_B^2 - 1)(R_B - 1)(R_B - 2)}{R_B^2(2R_B - 1) + R_B^2(R_B^2 - 1) + R_B(R_B^2 - 1)(R_B - 1)} \quad (\text{eq. A5.16})$$

$$p_{23} = \frac{R_B - 2}{2R_B - 1} + \frac{2}{R_B} \quad (\text{eq. A5.17})$$

$$p_{24} = \frac{R_B - 1}{R_B(2R_B - 1)} \times (R_B - 2) \quad (\text{eq. A5.18})$$

$$P_{34} = 1$$

And the possible paths S_i of water for the 4th order catchment are:

Path S1 : a1->r1->r2-> r3 -> r4 -> outlet;

Path S2 : a1->r1-> r3 -> r4 ->outlet;

Path S3 : a1 ->r1-> r4 -> outlet;

Path S4 : a2 -> r2-> r3-> r4 -> outlet;

Path S5 : a2-> r2 -> r4 -> outlet;

Path S6 : a3-> r3-> r4 -> outlet;

Path S7 : a4 -> r4 -> outlet.

3. Convolution of nonidentical exponential probability density function of a given path S_i can be obtained as²:

$$f_{S_i} = f_{Tai}(t) \times f_{Tri}(t) \times f_{Tri+1}(t) \times \dots \times f_{Tr\Omega}(t) = \sum_{j=1}^{\Omega} \frac{\lambda_i \dots \lambda_{\Omega-1} \exp(-\lambda_j t)}{[(\lambda_i - \lambda_j) \dots (\lambda_{j-1} - \lambda_j) (\lambda_{j+1} - \lambda_j) \dots (\lambda_{\Omega} - \lambda_j)]} \quad (\text{eq. A5.19})$$

² See Bras, R.L., 1990. Hydrology: An introduction to hydrologic science. Addison-Wesley series in Civil Engineering. Addison-Wesley, 643 pp. (p.616)

5.2. Simulation results

5.2.1. Sensitivity analysis

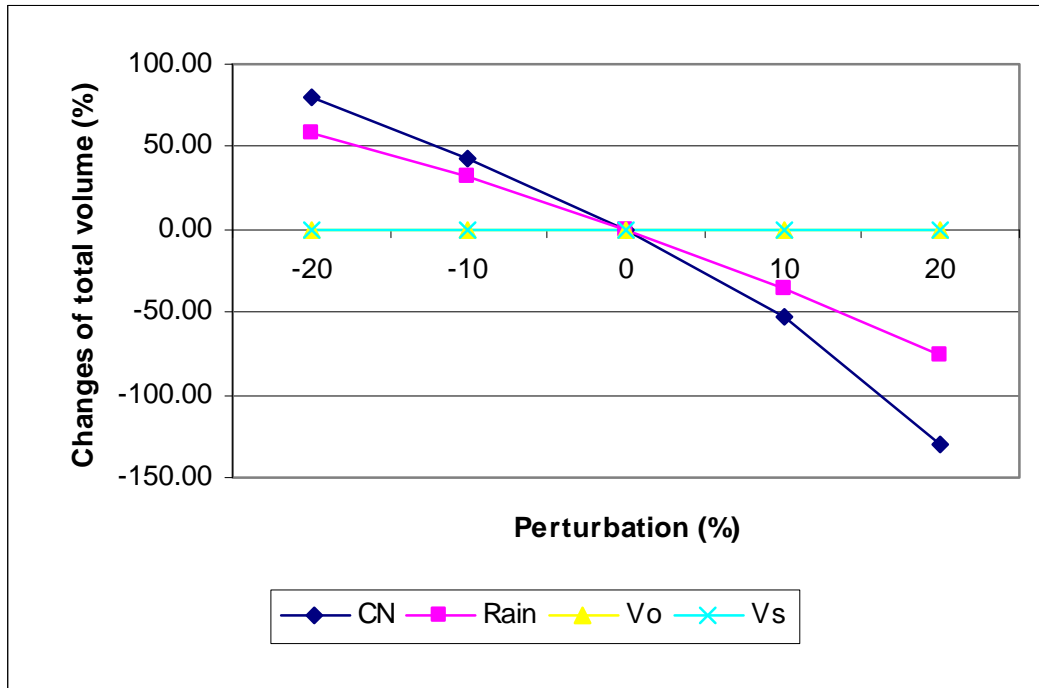


Figure A5.1: Sensitivity analysis for flow discharge (Hydrological parameters)

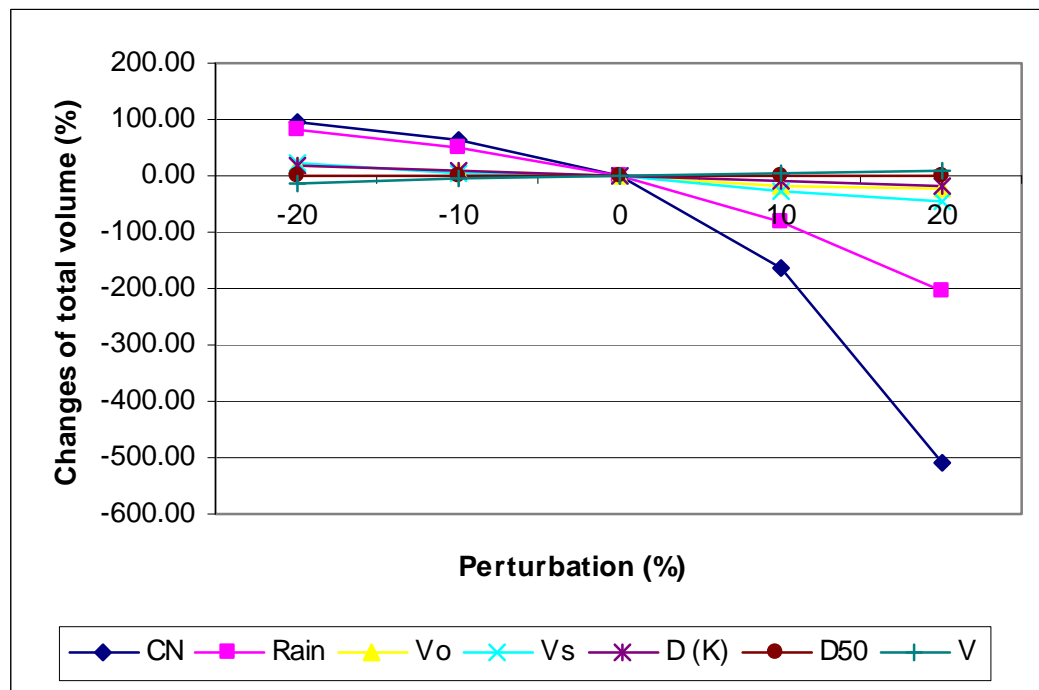


Figure A5.2: Sensitivity analysis for sediment (hydrological and soil erosion parameters)

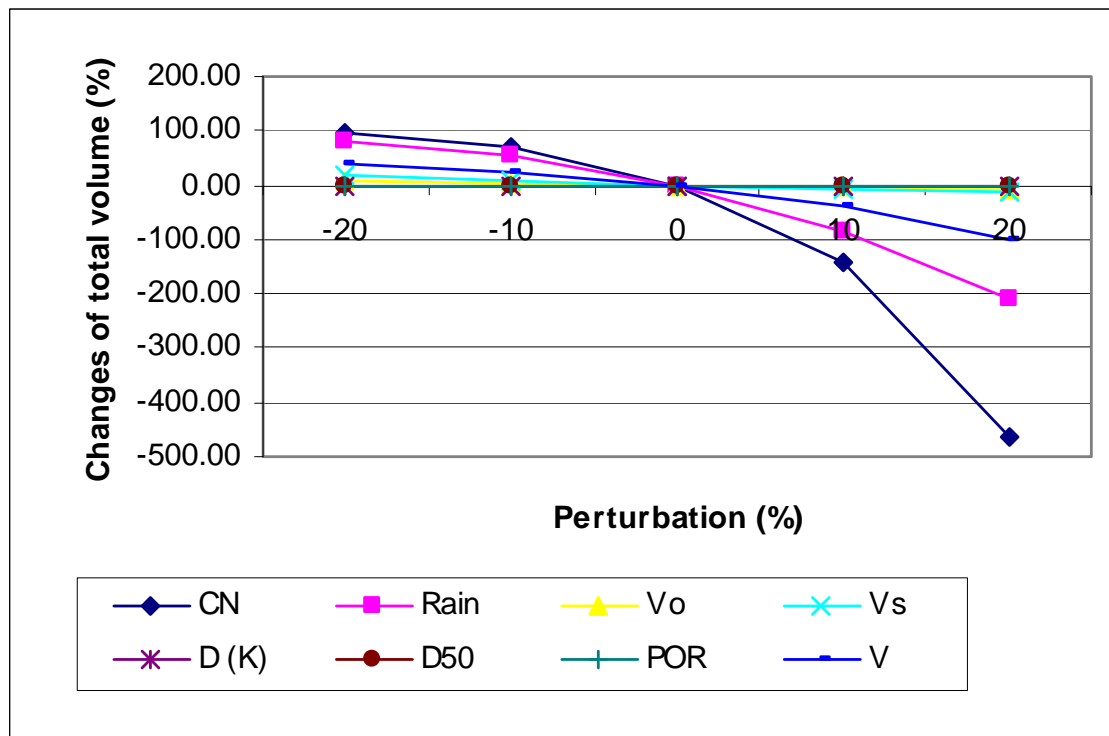


Figure A5.3: Sensitivity analysis for nutrients (hydrological and soil erosion parameters)

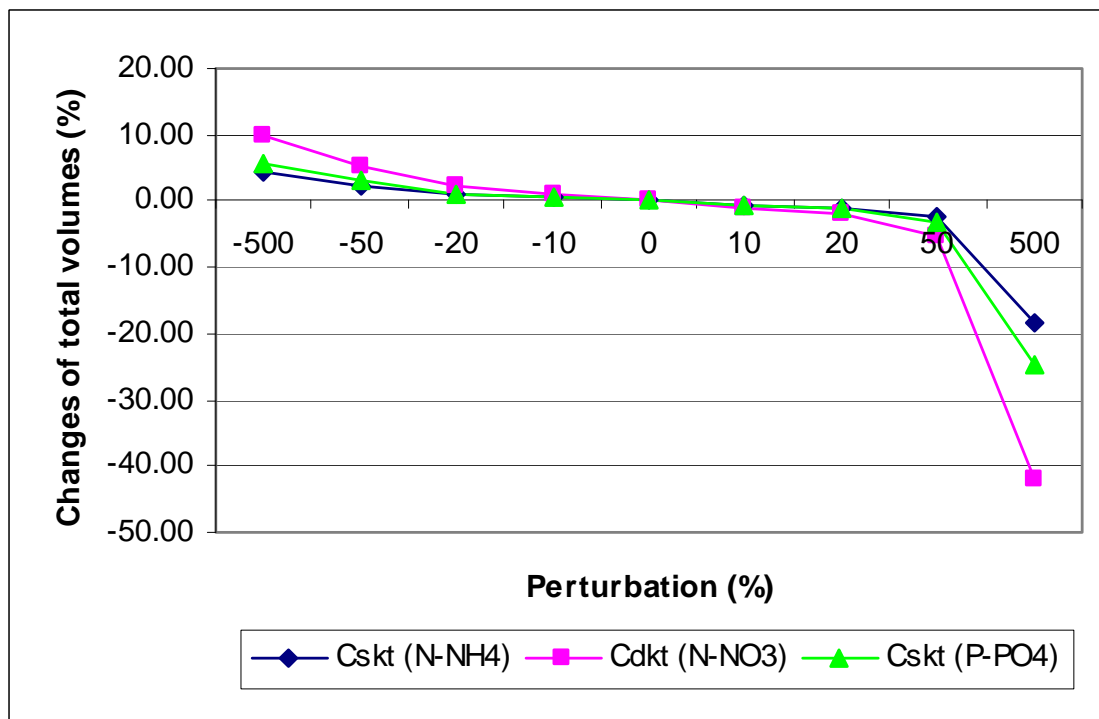


Figure A5.4: Sensitivity analysis for nutrients (using nutrient loading parameters)

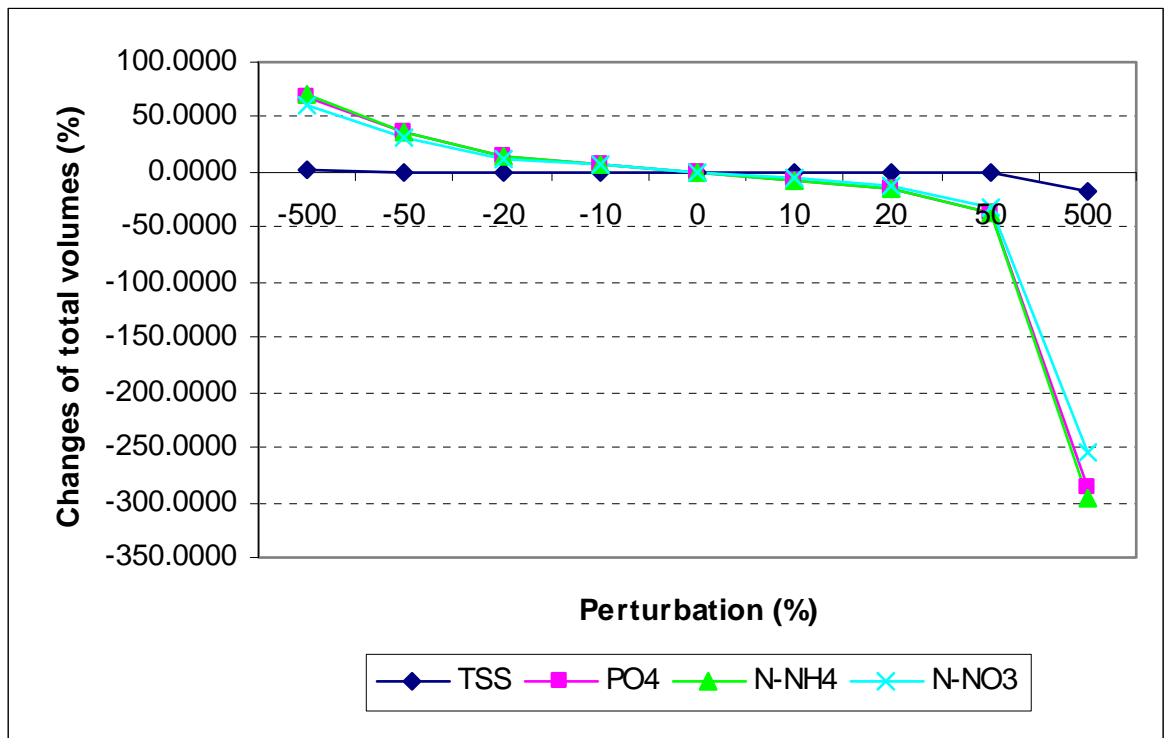


Figure A5.5: Sensitivity analysis for nutrients (using point sources)

5.2.2. Model results

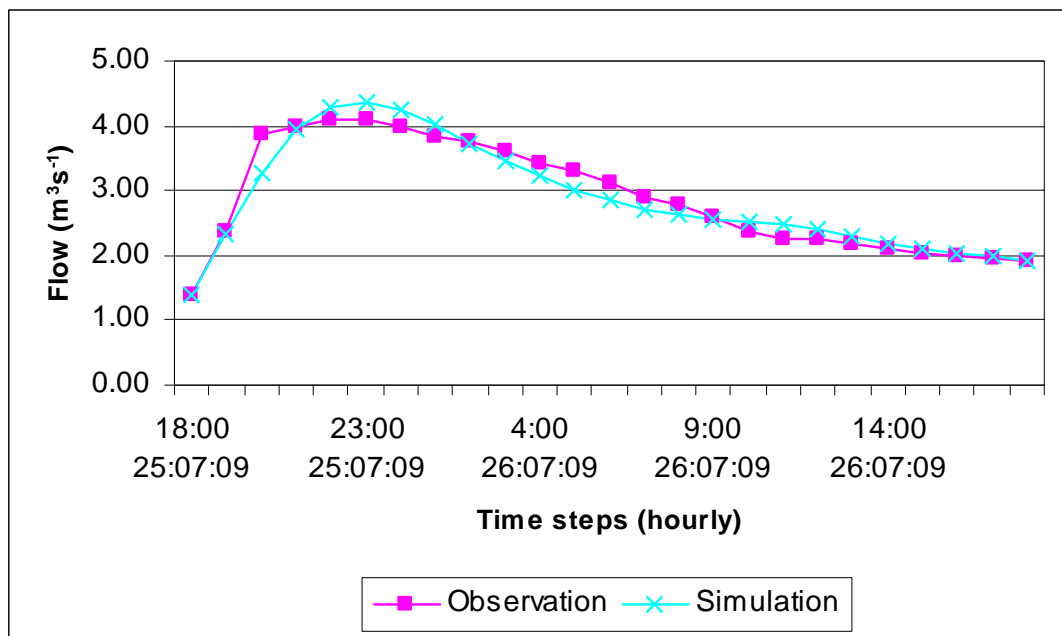


Figure A5.6: Observed and simulated flow discharge (including baseflow and interflow)

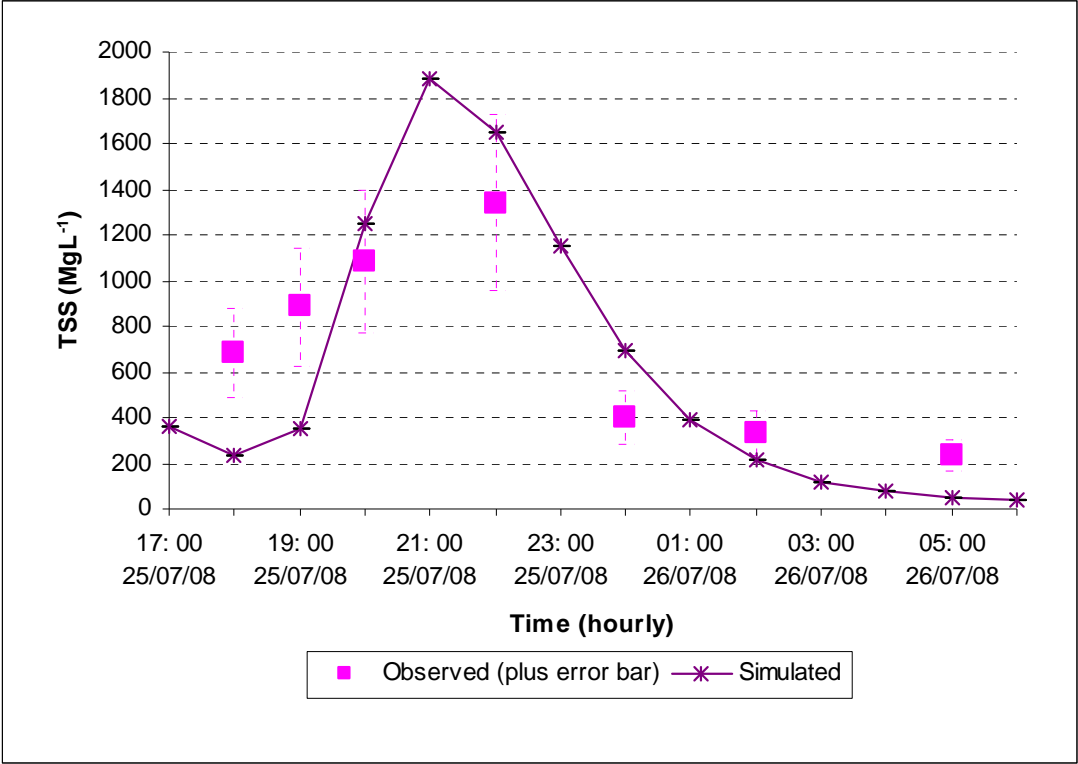


Figure A5.7: Observed and simulated suspended solid

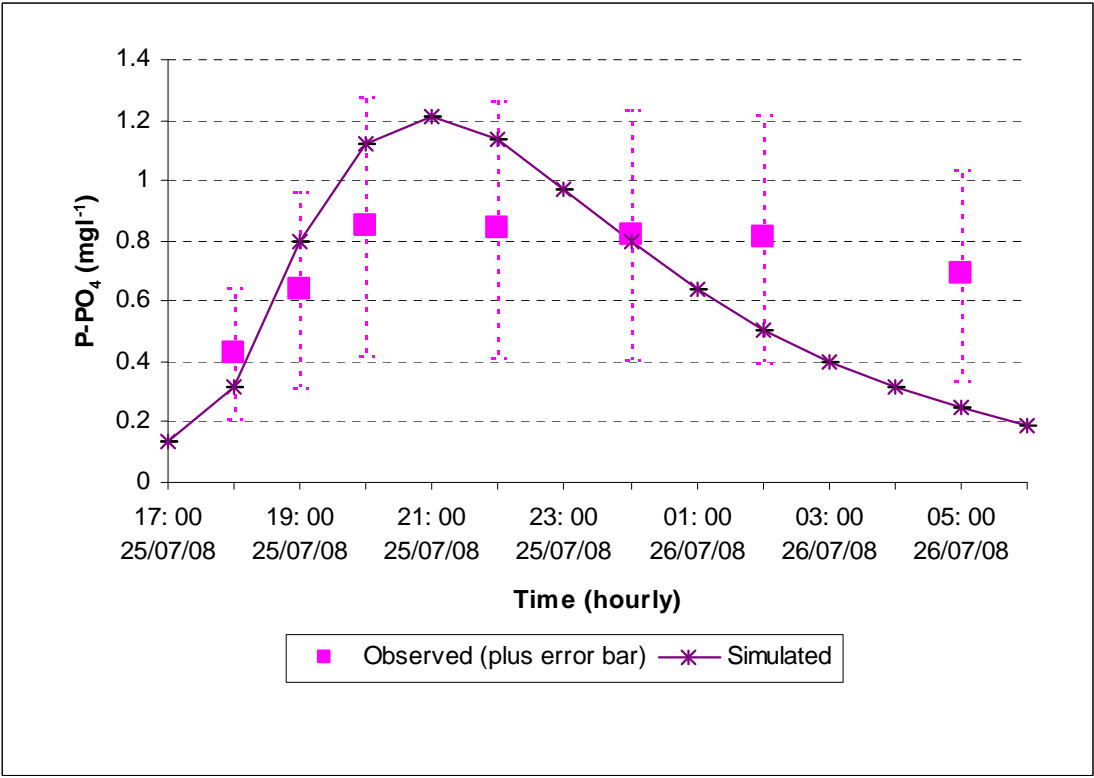


Figure A5.8: Observed and simulated P-PO4

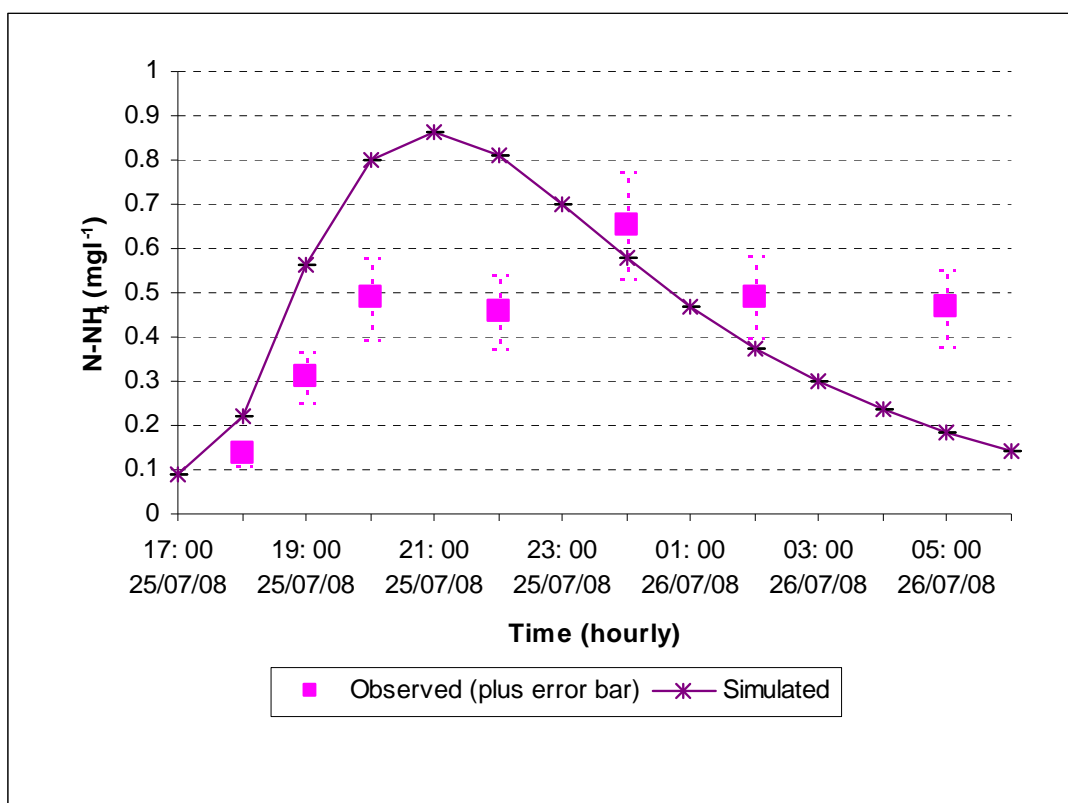


Figure A5.9: Observed and simulated N-NH₄

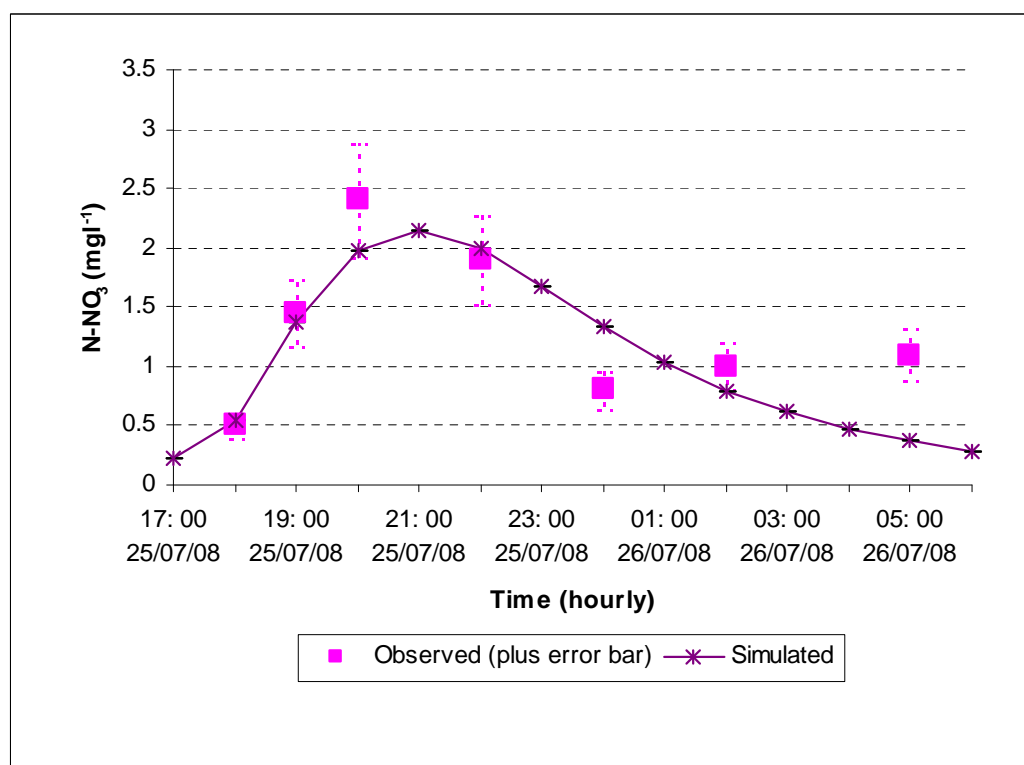


Figure A5.10: Observed and simulated N-NO₃

5.2.3. Model uncertainty

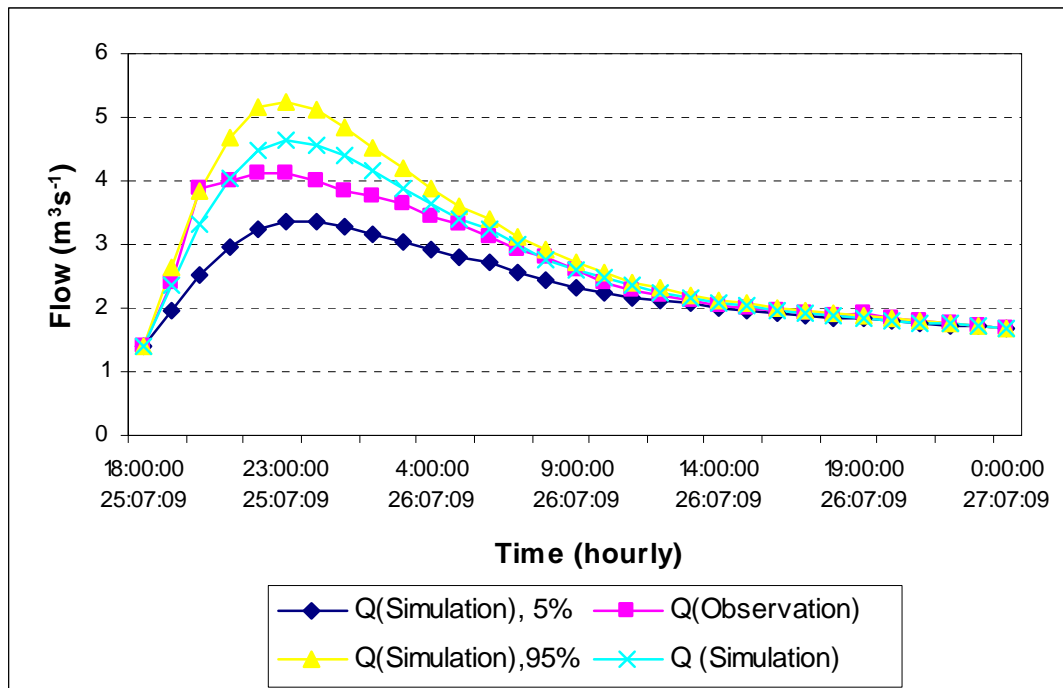


Figure A5.11: Flow simulation results (NSE:0.85 – 0.95)

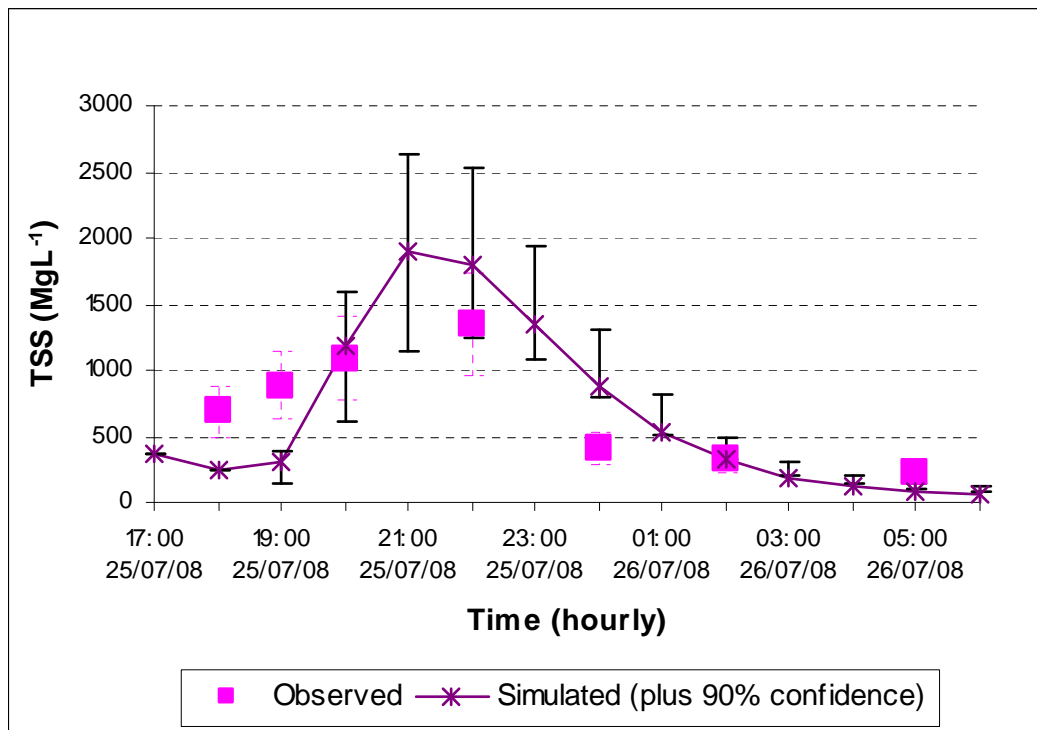


Figure A5.12: TSS simulation results

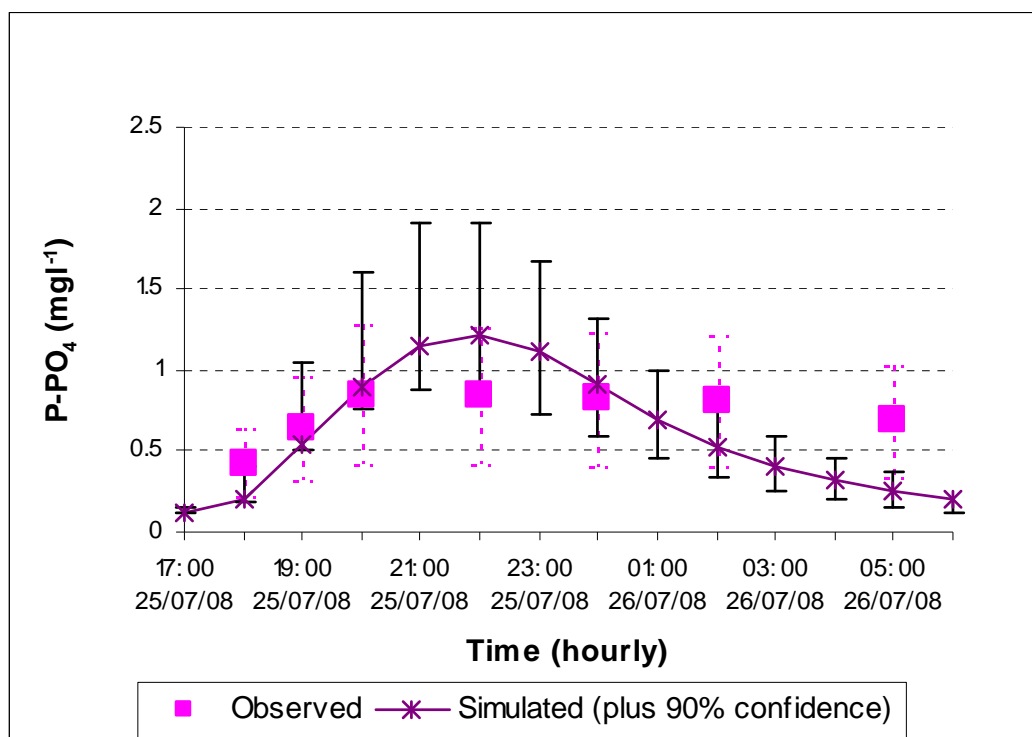


Figure A5.13: Phosphorus phosphate (P-PO₄) simulation results

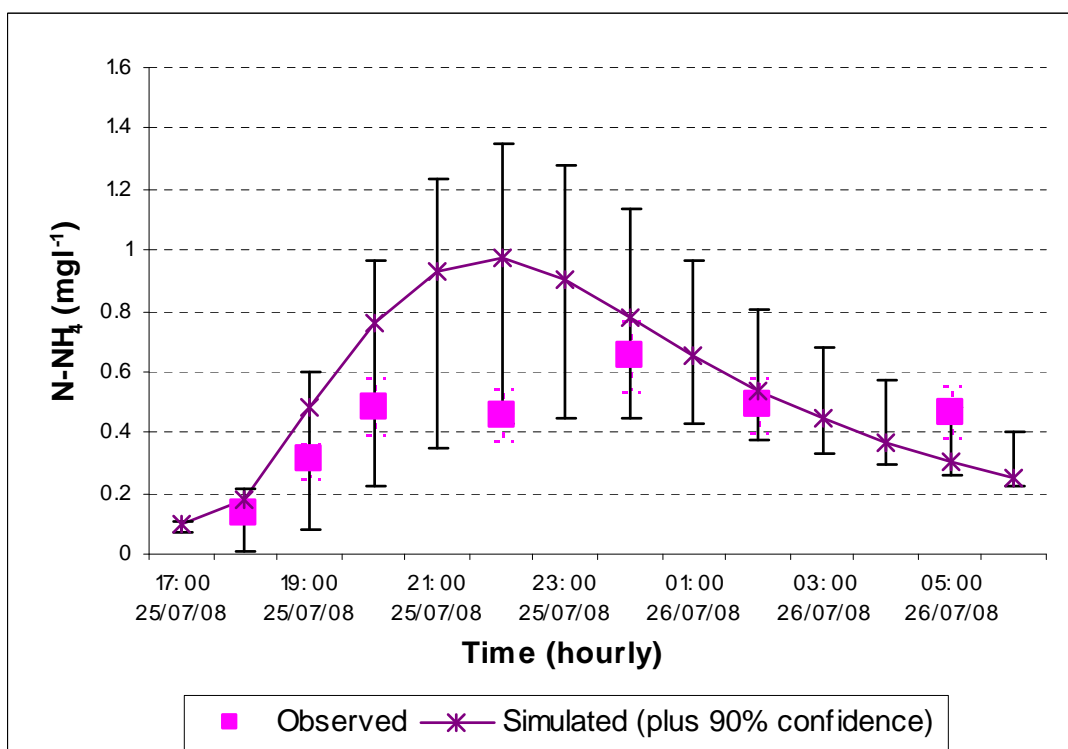


Figure A5.14: Nitrogen ammonium (N-NH₄) simulation results

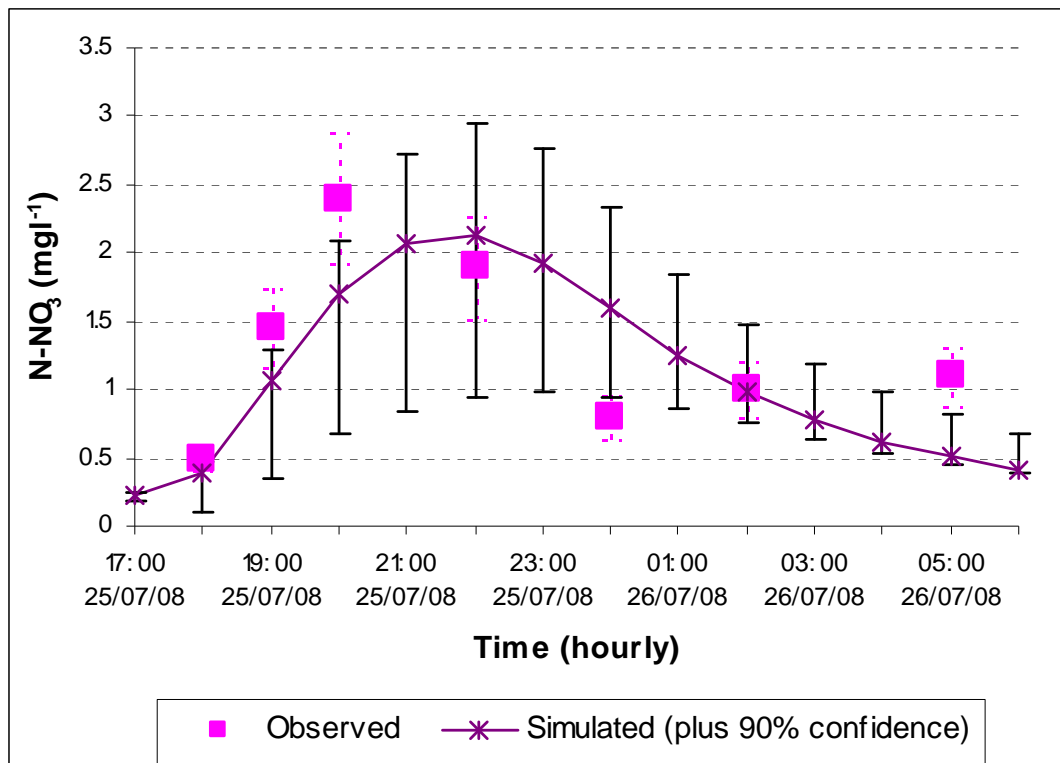


Figure A5.15: Nitrogen nitrate (N-NO₃) simulation results

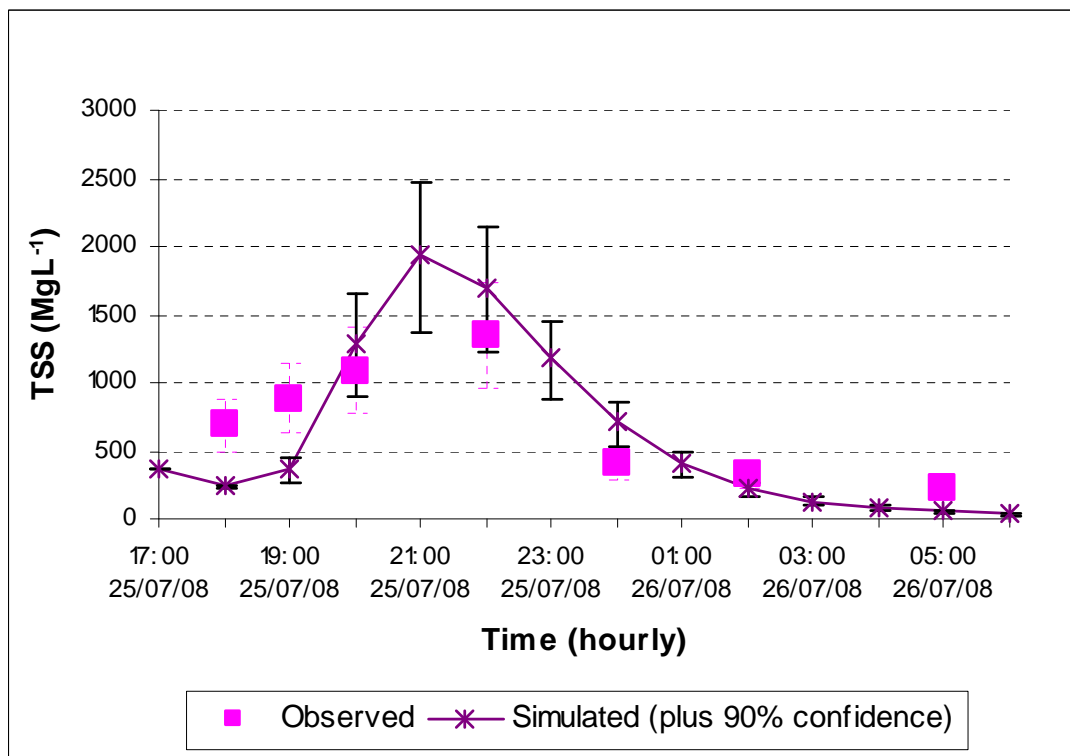


Figure A5.16: TSS simulation results (without CN, rainfall, V_{river})

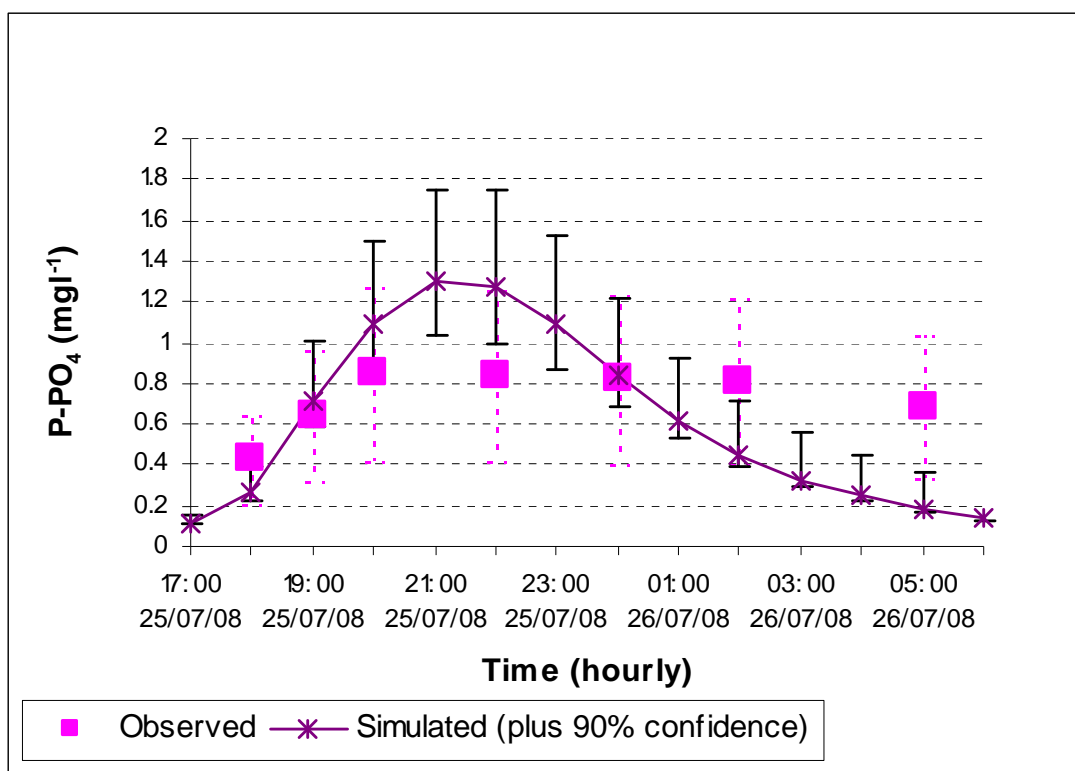


Figure A5.17: Phosphorus phosphate (P-PO₄) simulation results (without CN, rainfall, V_river)

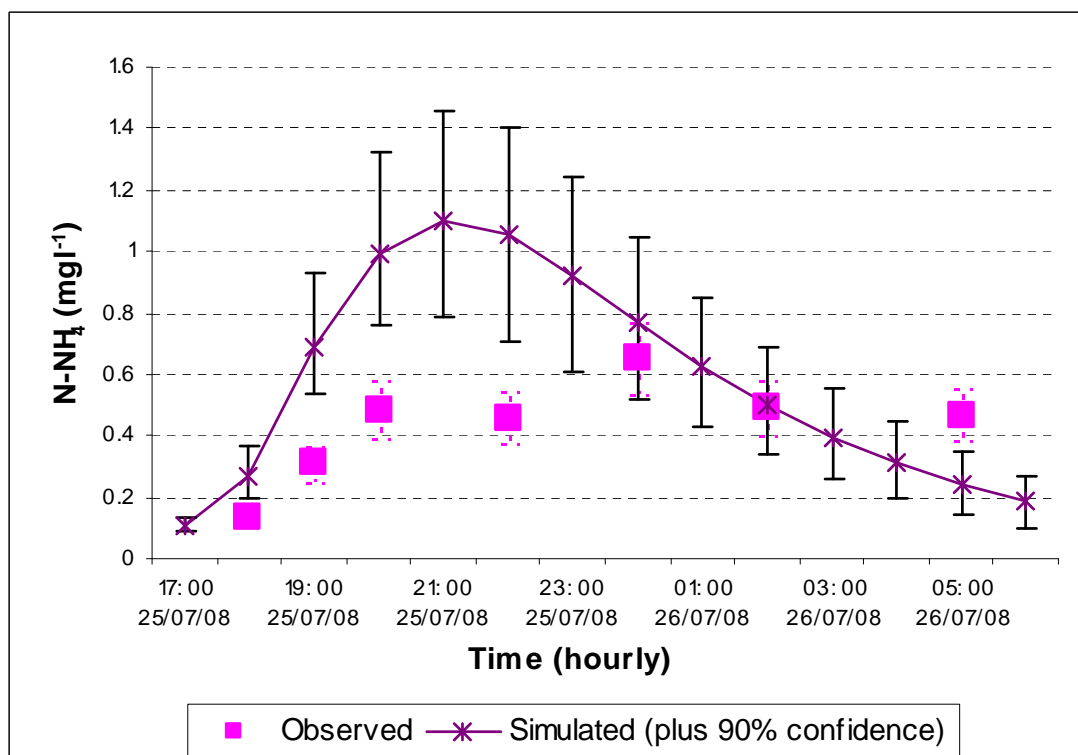


Figure A5.18: Nitrogen ammonium (N-NH₄) simulation results (without CN, rainfall, V_river)

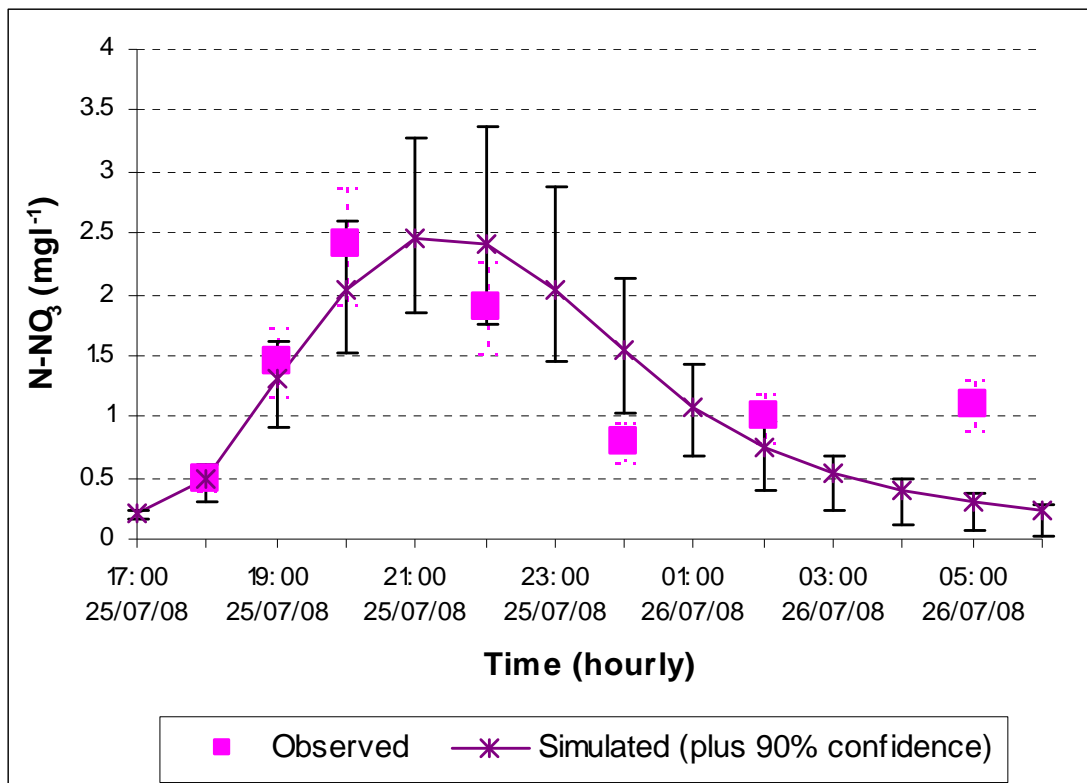


Figure A5.19: Nitrogen nitrate (N-NO₃) simulation results (without CN, rainfall, V_{river})

6. Appendix 6: Model parameters of the simplified process (SP) model for sediment yield

Table A6.1: Land classes schemes (León, 1999)

<i>ClassNo</i>	<i>ClassType</i>	<i>Typical Land Code</i>	<i>GC</i>	<i>CF</i>
Class 6	Impervious	UrRe	0.1	0.9
	Bareground	UrGd	0.1	0.9
	Forests	NUWod	0.8	0.4
	Crops LowVeg	NUSg	0.5	0.6
	Wetlands	NUWe	0.6	0.5
	Water	NUWa	0	0
Class 10	Impervious	UrRe	0.1	0.9
	Bareground Light	NUff	0.1	0.9
	Bareground Dark	UrTs	0.2	0.85
	Forests Light	NUWol	0.8	0.35
	Forests Dense	NUWod	0.9	0.3
	Grass	NUGr	0.5	0.6
	Crops Low	NUSg	0.6	0.5
	Crops High	NURc	0.7	0.4
	Wetlands	NUWe	0.6	0.5
	Water	NUWa	0	0

GC-Ground Cover Density ; CF-Canopy Cover Factor (Source Wischmeier and Smith, 1978)

Table A6.2: Soil type data table (León, 1999)

<i>SCS Code</i>	<i>Soil Class</i>	<i>HSC</i>	<i>SText</i>	<i>K</i>	<i>D₅₀</i>	<i>SpG</i>
s	sand	A	1	0.01	0.110	2.455
ls	loamy sand	A	1	0.05	0.130	2.293
sl	sandy loam	B	1	0.14	0.105	2.111
l	loam	B	2	0.31	0.075	2.009
sil	silt loam	C	2	0.37	0.035	2.099
si	silt	C	2	0.42	0.015	1.920
scl	sandy clay loam	B	1	0.22	0.330	1.949
cl	clay loam	C	3	0.29	0.310	1.857
sicl	silty clay loam	C	2	0.31	0.038	1.977
sc	sandy clay	B	1	0.15	0.550	1.849
sic	silty clay	C	3	0.24	0.100	1.920
c	clay	D	3	0.20	0.610	1.840

HSC-Soil Group; SText-Soil Texture; K-K factor; D₅₀ -Median Particle Size; SpG - Specific Weight